

Validation of Protein NMR Chemical Shift Assignments against NOE Data

Areca (v. 1.00) @ NMRFAM

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Abstract

This comprehensive report provides the calculated probabilities and the reasoning behind the calculations. This validation report contains three sections.

Disclaimer (Section 1)

Graphical overall report (Section 2):

Overall 2D plot (subsection 2.1): This figure shows a scatter plot of probabilities v.s. confidences of the residues.

Overall report per residue (subsection 2.2): In order to show the overall probabilities for every residue, ARECA considers the probabilities of N, CA, and CB to calculate the overall backbone (plus CB) probabilities. These overall backbone probabilities are displayed as a bar graph. In addition, a second graph displays the overall proton probability of every residue.

Overall report per atom (subsection 2.3): This report consists of a set of plots showing the probabilities of all the assigned atoms. In these plots, the residues are distributed along the x-axis and every atom is labeled and color-coded based its overall probability.

Detailed report for atoms (list of residues 3):

This section provides more details about the calculated probabilities for every residue.

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1 disclaimer

Areca @ NMRFAM

Please note that usage of the ARECA package should be acknowledged in any publication.

The program is provided as is, and the NMRFAM and/or the developers are not responsible for the outcomes of any kind of these results.

For any question or concern please contact ARECA.nmrfam@gmail.com.

2 Overall Reports

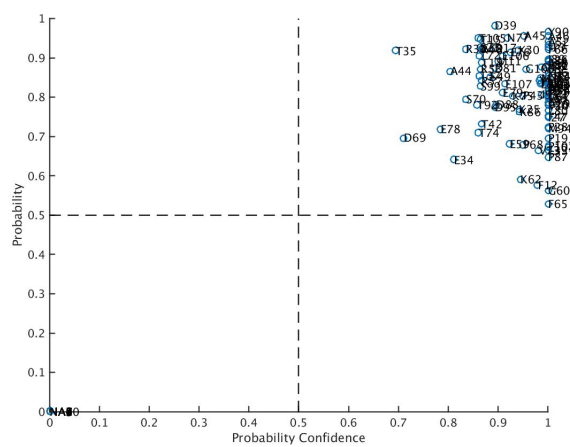
Figure: Overall 2D probabilities v.s. confidences2.1

Figures: Overall probabilities2.2

Figures: Probabilities of atoms for every residue2.3

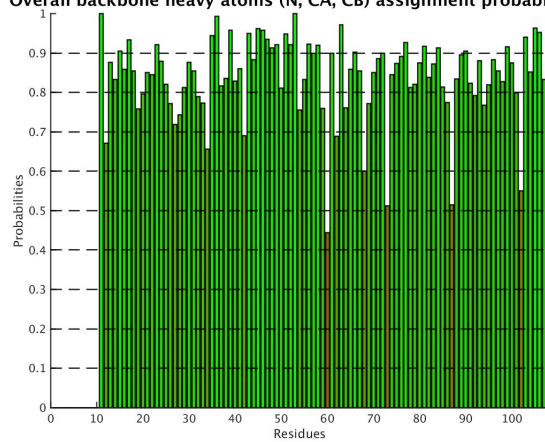
2.1 Overall 2D probabilities v.s. confidences

In ideal cases all the assigned residues should be in the top-right quadrant of the plot.

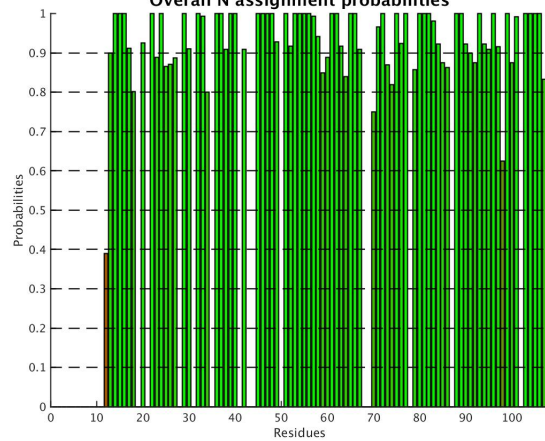


2.2 Figures: Overall Probabilities

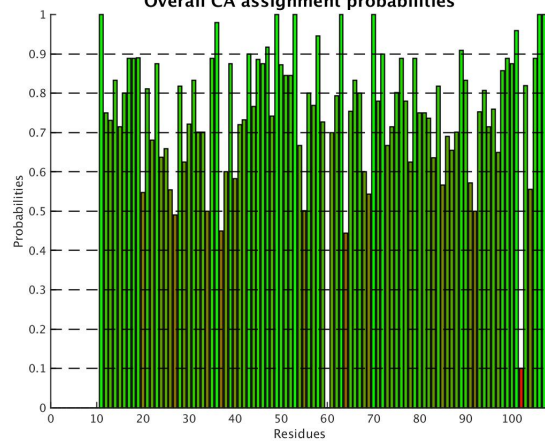
Overall backbone heavy atoms (N, CA, CB) assignment probabilities

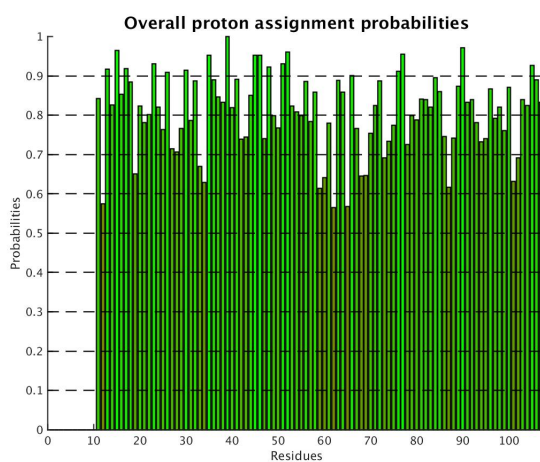
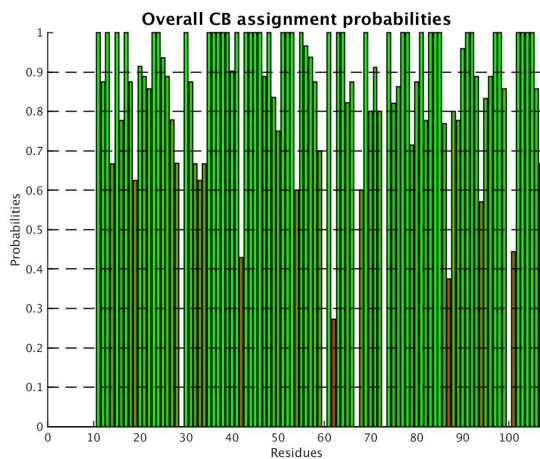


Overall N assignment probabilities

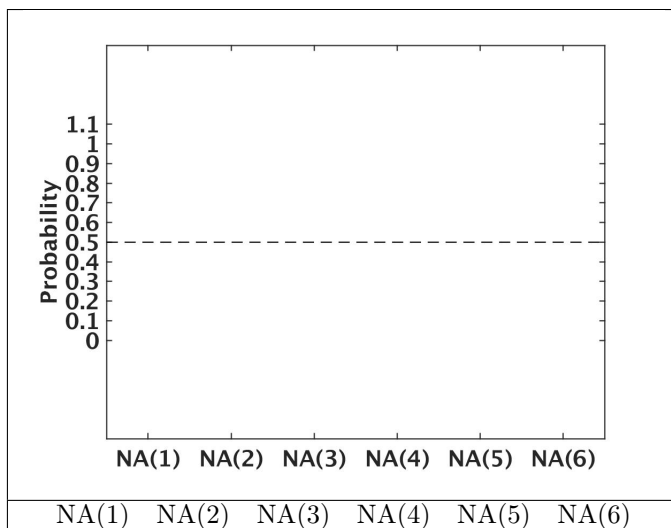


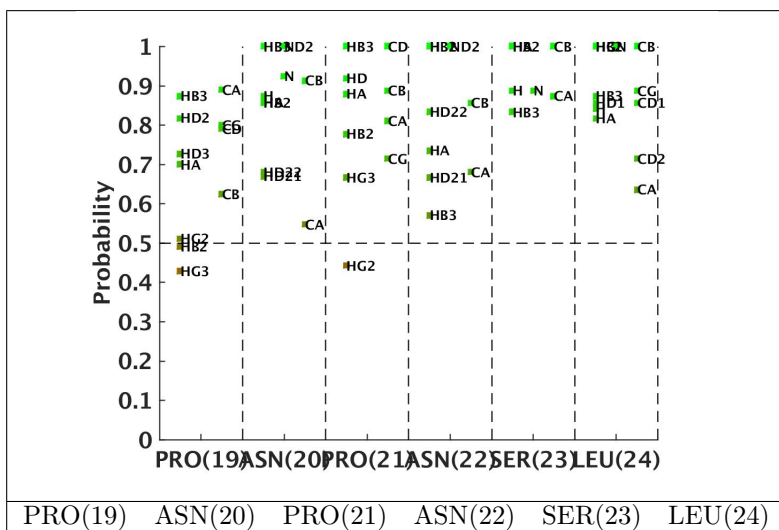
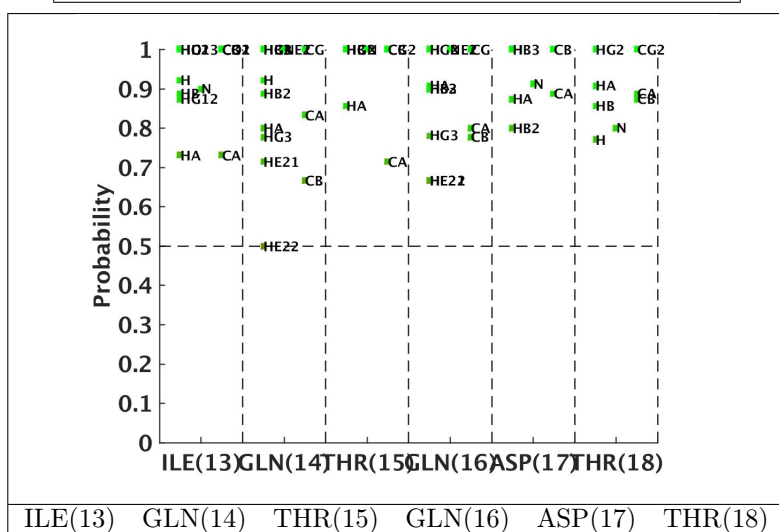
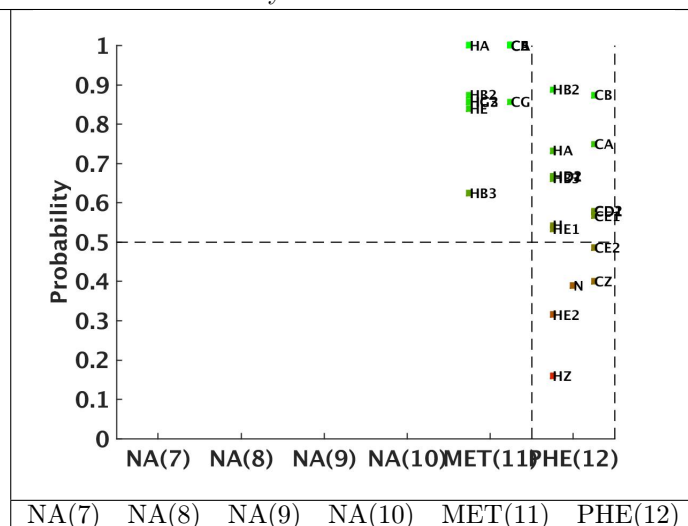
Overall CA assignment probabilities

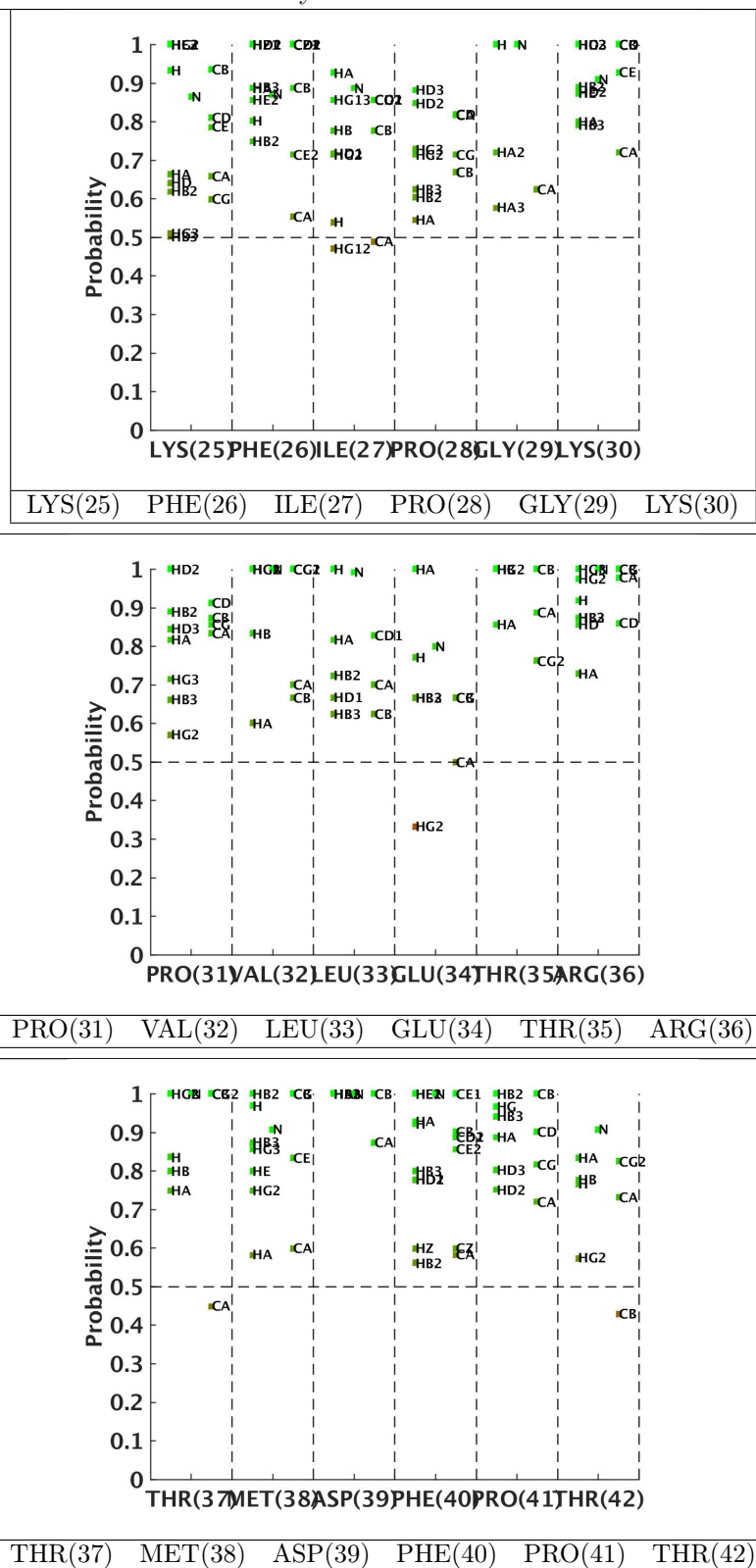


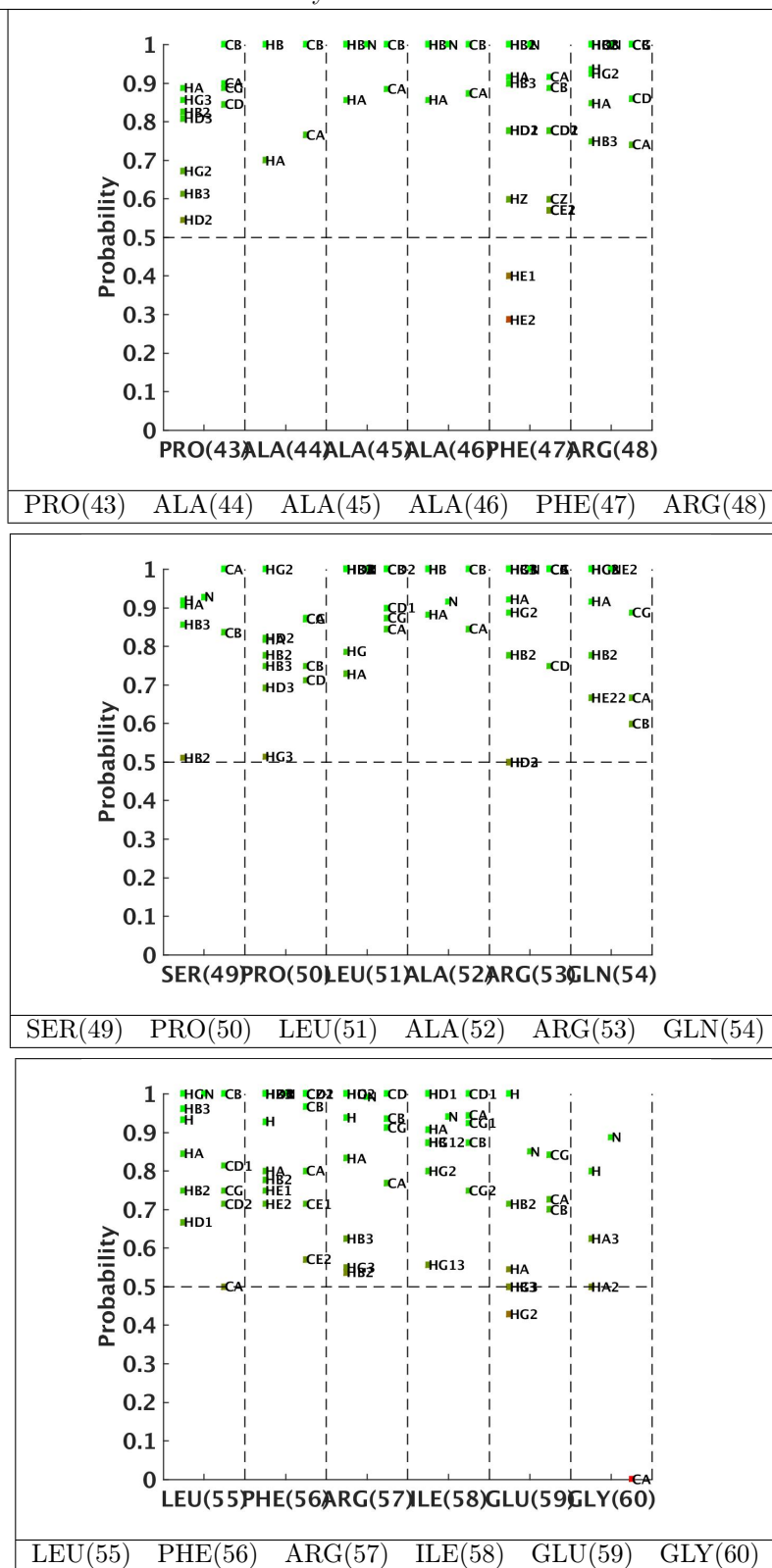


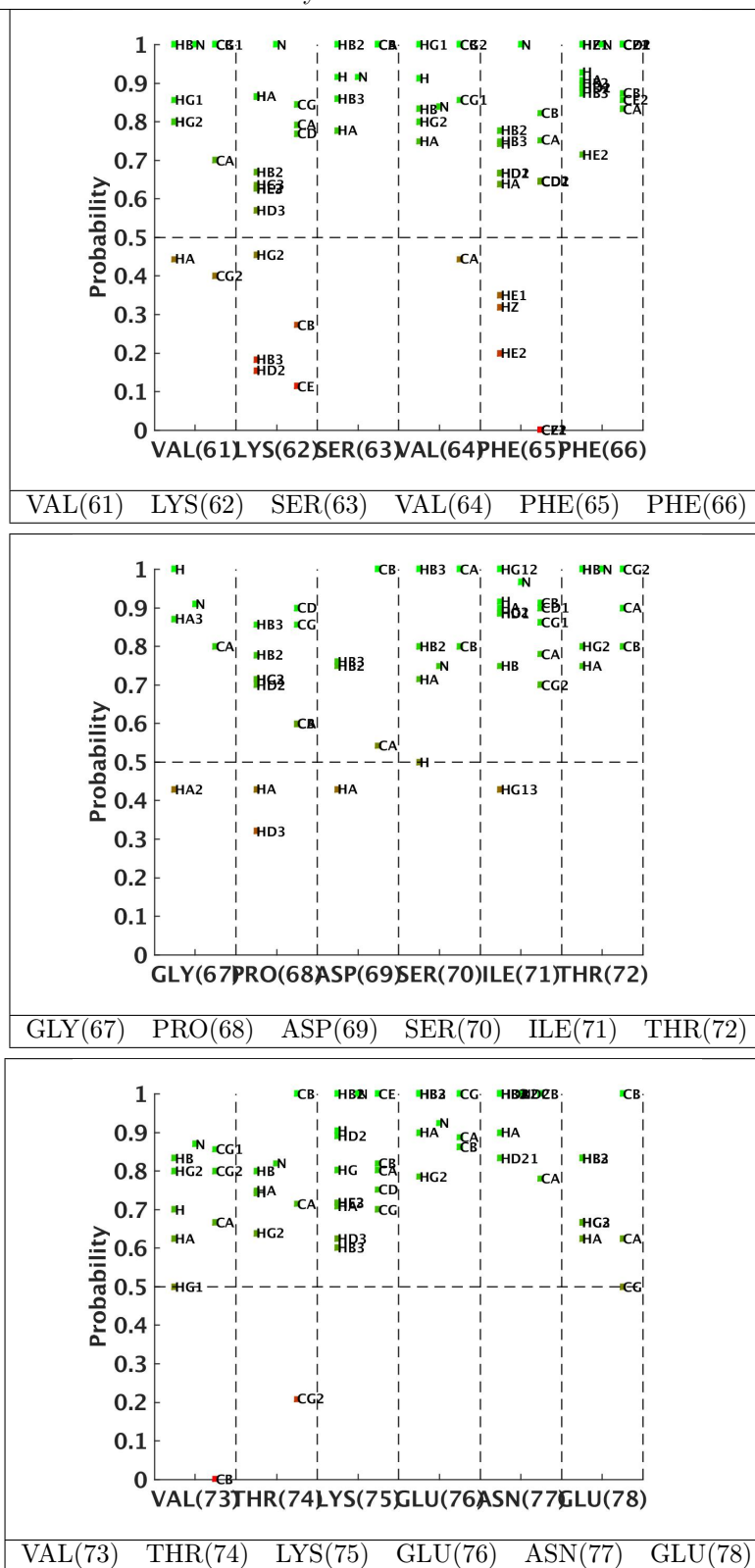
2.3 Figures: Probabilities of atoms for every residue

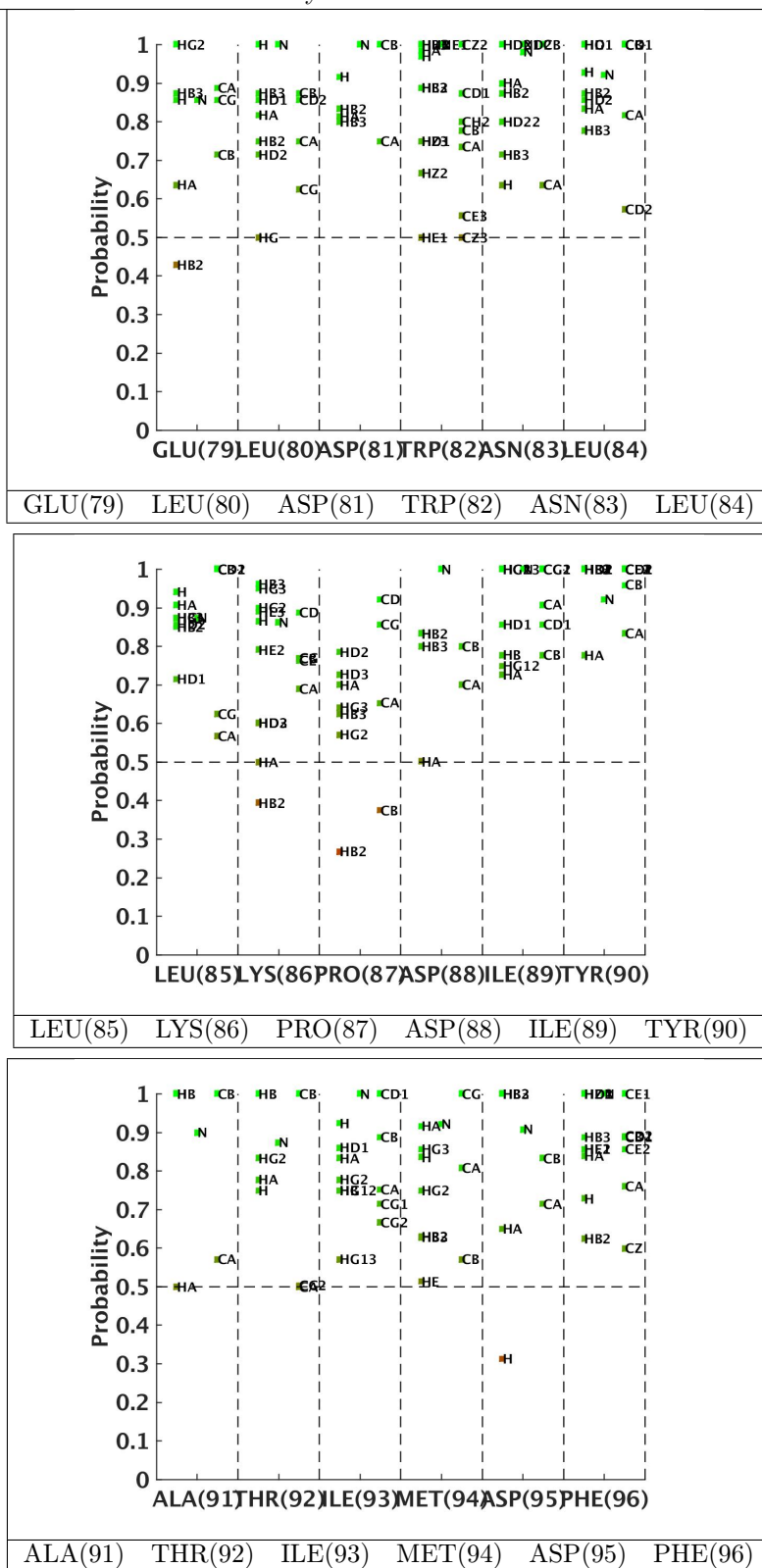


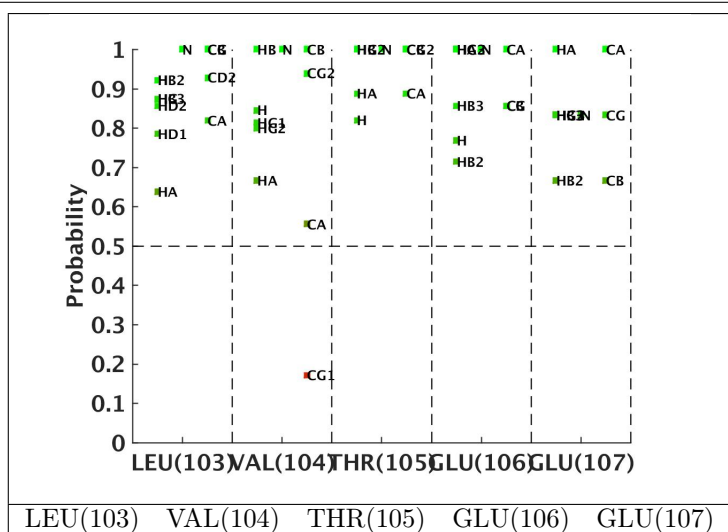
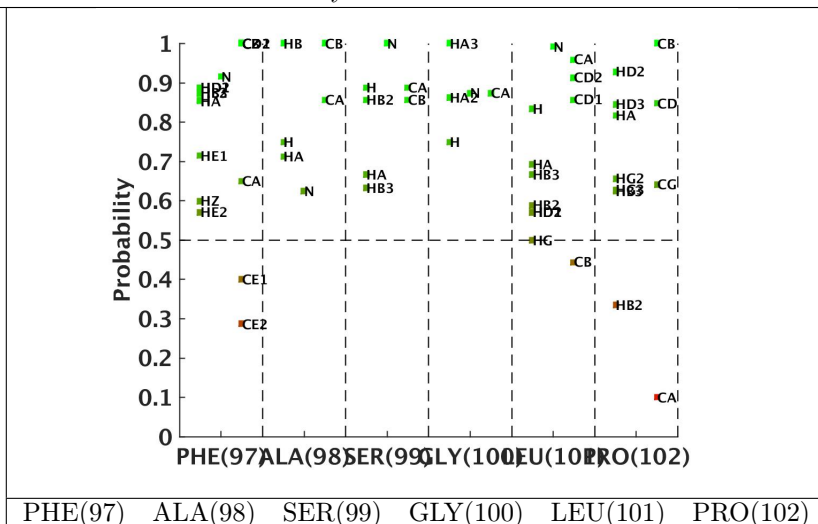












3 Residues Report

This section provides more details about the calculated probabilities. We considered a section for every residue, and the following table is linked to the sections.

| | | | | | |
|----------|----------|----------|----------|----------|----------|
| NA(1) | NA(2) | NA(3) | NA(4) | NA(5) | NA(6) |
| NA(7) | NA(8) | NA(9) | NA(10) | MET(11) | PHE(12) |
| ILE(13) | GLN(14) | THR(15) | GLN(16) | ASP(17) | THR(18) |
| PRO(19) | ASN(20) | PRO(21) | ASN(22) | SER(23) | LEU(24) |
| LYS(25) | PHE(26) | ILE(27) | PRO(28) | GLY(29) | LYS(30) |
| PRO(31) | VAL(32) | LEU(33) | GLU(34) | THR(35) | ARG(36) |
| THR(37) | MET(38) | ASP(39) | PHE(40) | PRO(41) | THR(42) |
| PRO(43) | ALA(44) | ALA(45) | ALA(46) | PHE(47) | ARG(48) |
| SER(49) | PRO(50) | LEU(51) | ALA(52) | ARG(53) | GLN(54) |
| LEU(55) | PHE(56) | ARG(57) | ILE(58) | GLU(59) | GLY(60) |
| VAL(61) | LYS(62) | SER(63) | VAL(64) | PHE(65) | PHE(66) |
| GLY(67) | PRO(68) | ASP(69) | SER(70) | ILE(71) | THR(72) |
| VAL(73) | THR(74) | LYS(75) | GLU(76) | ASN(77) | GLU(78) |
| GLU(79) | LEU(80) | ASP(81) | TRP(82) | ASN(83) | LEU(84) |
| LEU(85) | LYS(86) | PRO(87) | ASP(88) | ILE(89) | TYR(90) |
| ALA(91) | THR(92) | ILE(93) | MET(94) | ASP(95) | PHE(96) |
| PHE(97) | ALA(98) | SER(99) | GLY(100) | LEU(101) | PRO(102) |
| LEU(103) | VAL(104) | THR(105) | GLU(106) | GLU(107) | |

3.1 NA(1)

3.2 NA(2)

3.3 NA(3)

3.4 NA(4)

3.5 NA(5)

3.6 NA(6)

3.7 NA(7)

3.8 NA(8)

3.9 NA(9)

3.10 NA(10)

3.11 MET(11)

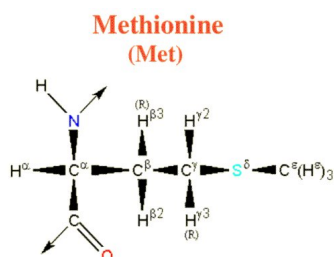


Figure 1: Image from the BMRB

Residue probability: 0.891

Residue probability confidence: 0.900

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | NA | – | – | 0.000 | 0.000 |
| CA 3.11.1 | 55.594 | 56.303 | 4.222 | 1.000 | 0.875 |
| CB 3.11.2 | 31.532 | 33.217 | 4.564 | 1.000 | 0.875 |
| CG 3.11.3 | 33.719 | 32.123 | 4.122 | 0.857 | 0.875 |
| CE 3.11.4 | 16.766 | 17.286 | 5.508 | 1.000 | 1.000 |
| N | NA | – | – | 0.000 | 0.000 |
| HA 3.11.5 | 4.255 | 4.409 | 0.504 | 1.000 | 0.875 |
| HB2 3.11.6 | 2.197 | 2.016 | 0.340 | 0.875 | 0.875 |
| HB3 3.11.7 | 2.311 | 1.978 | 0.359 | 0.625 | 0.875 |
| HG2 3.11.8 | 1.795 | 2.410 | 0.360 | 0.857 | 0.875 |
| HG3 3.11.9 | 1.786 | 2.378 | 0.386 | 0.857 | 0.875 |
| HE 3.11.10 | 1.791 | 1.877 | 0.381 | 0.839 | 1.000 |
| H | NA | – | – | 0.000 | 0.000 |

3.11.1 Detailed Probabilities of MET11CA:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET11 | 1.00 | 0.83 |
| PHE12 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M11HB2 | 1.00 |
| M11HB3 | 1.00 |
| M11HG2 | 1.00 |
| M11HG3 | 1.00 |
| M11H | 1.00 |
| M11HA | 1.00 |
| F12HA | 1.00 |
| F12H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET11 | HA | 1.00 | 0.004 | 1.00 | 11.73 |
| MET11 | HB2 | 1.00 | 0.007 | 1.00 | 0.47 |
| MET11 | HB3 | 1.00 | 0.005 | 1.00 | 0.41 |
| MET11 | HG2 | 1.00 | 0.007 | 1.00 | 1.51 |
| MET11 | HG3 | 1.00 | 0.002 | 1.00 | 1.51 |
| MET11 | HE1 | 0.69 | 0.003 | 1.00 | 1.51 |
| PHE12 | HA | 1.00 | 0.013 | 1.00 | 0.06 |
| PHE12 | H | 1.00 | 0.002 | 1.00 | 0.41 |

3.11.2 Detailed Probabilities of MET11CB:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET11 | 1.00 | 0.86 |
| PHE12 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M11HA | 1.00 |
| M11HB3 | 1.00 |
| M11HG2 | 1.00 |
| M11HG3 | 1.00 |
| M11HE1 | 0.96 |
| M11H | 1.00 |
| M11HB2 | 1.00 |
| F12H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET11 | HA | 1.00 | 0.002 | 1.00 | 0.35 |
| MET11 | HB2 | 1.00 | 0.004 | 1.00 | 13.20 |
| MET11 | HB3 | 1.00 | 0.008 | 1.00 | 6.70 |
| MET11 | HG2 | 1.00 | 0.006 | 1.00 | 1.20 |
| MET11 | HG3 | 1.00 | 0.003 | 1.00 | 1.20 |
| MET11 | HE1 | 0.96 | 0.002 | 1.00 | 1.20 |
| PHE12 | H | 1.00 | 0.012 | 1.00 | 0.09 |

3.11.3 Detailed Probabilities of MET11CG:

Overall probability: 0.857

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET11 | 0.83 | 0.86 |
| PHE12 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M11HA | 1.00 |
| M11HB2 | 1.00 |
| M11HB3 | 1.00 |
| M11HG2 | 1.00 |
| M11HE1 | 1.00 |
| M11H | 1.00 |
| M11HG3 | 1.00 |
| F12H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET11 | HA | 1.00 | 0.000 | 1.00 | 0.70 |
| MET11 | HB2 | 1.00 | 0.005 | 1.00 | 0.56 |
| MET11 | HB3 | 1.00 | 0.109 | 0.00 | 0.00 |
| MET11 | HG2 | 1.00 | 0.008 | 1.00 | 14.05 |
| MET11 | HG3 | 1.00 | 0.001 | 1.00 | 14.05 |
| MET11 | HE1 | 1.00 | 0.004 | 1.00 | 14.05 |
| PHE12 | H | 0.97 | 0.012 | 1.00 | 0.06 |

3.11.4 Detailed Probabilities of MET11CE:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET11 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M11HB2 | 0.96 |
| M11HB3 | 0.97 |
| M11HG2 | 1.00 |
| M11HG3 | 1.00 |
| M11HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET11 | HB2 | 0.96 | 0.002 | 1.00 | 0.31 |
| MET11 | HB3 | 0.97 | 0.008 | 1.00 | 0.41 |
| MET11 | HG2 | 1.00 | 0.004 | 1.00 | 138.78 |
| MET11 | HG3 | 1.00 | 0.005 | 1.00 | 138.78 |
| MET11 | HE1 | 1.00 | 0.000 | 1.00 | 138.78 |
| MET11 | HA | 0.67 | 0.014 | 1.00 | 0.38 |

3.11.5 Detailed Probabilities of MET11HA:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET11 | 1.00 | 0.83 |
| PHE12 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M11HB2 | 1.00 |
| M11HB3 | 1.00 |
| M11HG2 | 1.00 |
| M11HG3 | 1.00 |
| M11H | 1.00 |
| M11HA | 1.00 |
| F12HA | 1.00 |
| F12H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET11 | HA | 1.00 | 0.004 | 1.00 | 11.73 |
| MET11 | HB2 | 1.00 | 0.002 | 1.00 | 0.35 |
| MET11 | HB3 | 1.00 | 0.007 | 1.00 | 0.74 |
| MET11 | HG2 | 1.00 | 0.000 | 1.00 | 0.70 |
| MET11 | HG3 | 1.00 | 0.000 | 1.00 | 0.70 |
| MET11 | HE1 | 0.69 | 0.014 | 1.00 | 0.38 |
| PHE12 | HA | 1.00 | 0.017 | 1.00 | 0.14 |
| PHE12 | H | 1.00 | 0.004 | 1.00 | -263429.00 |

3.11.6 Detailed Probabilities of MET11HB2:

Overall probability: 0.875

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET11 | 1.00 | 0.86 |
| PHE12 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M11HA | 1.00 |
| M11HB3 | 1.00 |
| M11HG2 | 1.00 |
| M11HG3 | 1.00 |
| M11HE1 | 0.96 |
| M11H | 1.00 |
| M11HB2 | 1.00 |
| F12H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET11 | HA | 1.00 | 0.007 | 1.00 | 0.47 |
| MET11 | HB2 | 1.00 | 0.004 | 1.00 | 13.20 |
| MET11 | HB3 | 1.00 | 0.006 | 1.00 | 7.43 |
| MET11 | HG2 | 1.00 | 0.005 | 1.00 | 0.56 |
| MET11 | HG3 | 1.00 | 0.005 | 1.00 | 0.56 |
| MET11 | HE1 | 0.96 | 0.002 | 1.00 | 0.31 |
| PHE12 | H | 1.00 | 0.409 | 0.00 | 0.00 |
| PHE12 | HA | 0.67 | 0.004 | 1.00 | 0.11 |

3.11.7 Detailed Probabilities of MET11HB3:

Overall probability: 0.625

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET11 | 0.67 | 0.86 |
| PHE12 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M11HA | 1.00 |
| M11HB2 | 1.00 |
| M11HG2 | 1.00 |
| M11HG3 | 1.00 |
| M11HE1 | 0.97 |
| M11H | 1.00 |
| M11HB3 | 1.00 |
| F12H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET11 | HA | 1.00 | 0.005 | 1.00 | 0.41 |
| MET11 | HB2 | 1.00 | 0.008 | 1.00 | 6.70 |
| MET11 | HB3 | 1.00 | 0.005 | 1.00 | 21.15 |
| MET11 | HG2 | 1.00 | 0.109 | 0.00 | 0.00 |
| MET11 | HG3 | 1.00 | 0.109 | 0.00 | 0.00 |
| MET11 | HE1 | 0.97 | 0.008 | 1.00 | 0.41 |
| PHE12 | H | 1.00 | 0.523 | 0.00 | 0.00 |
| PHE12 | HA | 0.85 | 0.003 | 1.00 | 0.07 |

3.11.8 Detailed Probabilities of MET11HG2:

Overall probability: 0.857

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET11 | 0.83 | 0.86 |
| PHE12 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M11HA | 1.00 |
| M11HB2 | 1.00 |
| M11HB3 | 1.00 |
| M11HG3 | 1.00 |
| M11HE1 | 1.00 |
| M11H | 1.00 |
| M11HG2 | 1.00 |
| F12H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET11 | HA | 1.00 | 0.007 | 1.00 | 1.51 |
| MET11 | HB2 | 1.00 | 0.006 | 1.00 | 1.20 |
| MET11 | HB3 | 1.00 | 0.071 | 0.00 | 0.00 |
| MET11 | HG2 | 1.00 | 0.008 | 1.00 | 14.05 |
| MET11 | HG3 | 1.00 | 0.008 | 1.00 | 14.05 |
| MET11 | HE1 | 1.00 | 0.004 | 1.00 | 138.78 |
| PHE12 | H | 0.98 | 0.007 | 1.00 | -81657.00 |

3.11.9 Detailed Probabilities of MET11HG3:

Overall probability: 0.857

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET11 | 0.83 | 0.86 |
| PHE12 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M11HA | 1.00 |
| M11HB2 | 1.00 |
| M11HB3 | 1.00 |
| M11HG2 | 1.00 |
| M11HE1 | 1.00 |
| M11H | 1.00 |
| M11HG3 | 1.00 |
| F12H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET11 | HA | 1.00 | 0.002 | 1.00 | 1.51 |
| MET11 | HB2 | 1.00 | 0.003 | 1.00 | 1.20 |
| MET11 | HB3 | 1.00 | 0.062 | 0.00 | 0.00 |
| MET11 | HG2 | 1.00 | 0.001 | 1.00 | 14.05 |
| MET11 | HG3 | 1.00 | 0.001 | 1.00 | 14.05 |
| MET11 | HE1 | 1.00 | 0.005 | 1.00 | 138.78 |
| PHE12 | H | 0.97 | 0.002 | 1.00 | -81657.00 |

3.11.10 Detailed Probabilities of MET11HE1:

Overall probability: 0.839

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET11 | 0.84 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M11HB2 | 0.96 |
| M11HB3 | 0.97 |
| M11HG2 | 1.00 |
| M11HG3 | 1.00 |
| M11HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET11 | HB2 | 0.96 | 0.002 | 1.00 | 1.20 |
| MET11 | HB3 | 0.97 | 0.067 | 0.03 | 0.00 |
| MET11 | HG2 | 1.00 | 0.004 | 1.00 | 14.05 |
| MET11 | HG3 | 1.00 | 0.004 | 1.00 | 14.05 |
| MET11 | HE1 | 1.00 | 0.000 | 1.00 | 138.78 |
| MET11 | HA | 0.67 | 0.003 | 1.00 | 1.51 |

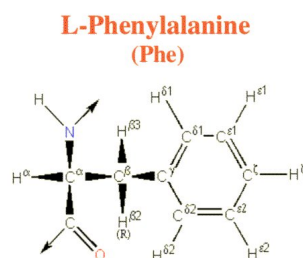
3.12 PHE(12)

Figure 2: Image from the BMRB

Residue probability: 0.576

Residue probability confidence: 0.980

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 173.858 | 175.508 | 2.010 | 0.000 | 0.000 |
| CA 3.12.1 | 57.236 | 58.245 | 3.808 | 0.750 | 0.900 |
| CB 3.12.2 | 39.949 | 40.078 | 3.616 | 0.875 | 1.000 |
| CD1 3.12.3 | 131.773 | 131.234 | 9.579 | 0.578 | 1.000 |
| CD2 3.12.4 | 131.845 | 131.352 | 9.581 | 0.579 | 1.000 |
| CE1 3.12.5 | 131.421 | 130.599 | 3.219 | 0.567 | 1.000 |
| CE2 3.12.6 | 131.667 | 130.633 | 2.839 | 0.486 | 1.000 |
| CZ 3.12.7 | 129.788 | 129.042 | 3.448 | 0.400 | 1.000 |
| N 3.12.8 | 121.868 | 120.315 | 4.931 | 0.389 | 0.929 |
| HA 3.12.9 | 4.641 | 4.625 | 1.237 | 0.733 | 0.900 |
| HB2 3.12.10 | 3.024 | 2.980 | 0.399 | 0.889 | 1.000 |
| HB3 3.12.11 | 2.977 | 2.916 | 0.434 | 0.663 | 1.000 |
| HD1 3.12.12 | 7.187 | 7.037 | 0.347 | 0.667 | 1.000 |
| HD2 3.12.13 | 7.187 | 7.022 | 0.417 | 0.668 | 1.000 |
| HE1 3.12.14 | 7.229 | 7.046 | 0.417 | 0.533 | 1.000 |
| HE2 3.12.15 | 7.229 | 7.043 | 0.400 | 0.315 | 1.000 |
| HZ 3.12.16 | 7.276 | 6.984 | 1.598 | 0.160 | 1.000 |
| H 3.12.17 | 8.451 | 8.375 | 0.710 | 0.543 | 0.929 |

3.12.1 Detailed Probabilities of PHE12CA:

Overall probability: 0.750

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET11 | 1.00 | 0.50 |
| PHE12 | 0.64 | 1.00 |
| ILE13 | 0.75 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M11HA | 1.00 |
| M11H | 0.96 |
| F12HB2 | 1.00 |
| F12HB3 | 1.00 |
| F12HD1 | 1.00 |
| F12HD2 | 1.00 |
| F12H | 1.00 |
| F12HA | 1.00 |
| I13H | 1.00 |
| I13HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET11 | HA | 1.00 | 0.017 | 1.00 | 0.14 |
| MET11 | HB2 | 0.67 | 0.004 | 1.00 | 0.11 |
| MET11 | HB3 | 0.85 | 0.003 | 1.00 | 0.07 |
| PHE12 | HA | 1.00 | 0.077 | 0.00 | 0.00 |
| PHE12 | HB2 | 1.00 | 0.012 | 1.00 | 0.68 |
| PHE12 | HB3 | 1.00 | 0.035 | 0.50 | 0.00 |
| PHE12 | HD1 | 1.00 | 0.017 | 1.00 | 0.27 |
| PHE12 | HD2 | 1.00 | 0.017 | 1.00 | 0.27 |
| PHE12 | H | 1.00 | 0.114 | 0.00 | 0.00 |
| PHE12 | HE1 | 0.74 | 0.025 | 1.00 | 0.30 |
| ILE13 | HA | 1.00 | 0.040 | 0.00 | 0.00 |
| ILE13 | H | 1.00 | 0.006 | 1.00 | 0.95 |
| ILE13 | HB | 0.53 | 0.020 | 1.00 | 0.13 |
| ILE13 | HG12 | 0.53 | 0.004 | 1.00 | 0.36 |

3.12.2 Detailed Probabilities of PHE12CB:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE12 | 0.86 | 1.00 |
| ILE13 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F12HA | 1.00 |
| F12HB2 | 1.00 |
| F12HD1 | 1.00 |
| F12HD2 | 1.00 |
| F12HE2 | 1.00 |
| F12H | 1.00 |
| F12HB3 | 1.00 |
| I13H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE12 | HA | 1.00 | 0.006 | 1.00 | 0.46 |
| PHE12 | HB2 | 1.00 | 0.028 | 1.00 | 4.41 |
| PHE12 | HB3 | 1.00 | 0.019 | 1.00 | 4.41 |
| PHE12 | HD1 | 1.00 | 0.000 | 1.00 | 0.49 |
| PHE12 | HD2 | 1.00 | 0.000 | 1.00 | 0.49 |
| PHE12 | HE2 | 1.00 | 0.042 | 0.00 | 0.00 |
| PHE12 | H | 1.00 | 0.004 | 1.00 | 0.09 |
| ILE13 | H | 1.00 | 0.013 | 1.00 | 0.10 |

3.12.3 Detailed Probabilities of PHE12CD1:

Overall probability: 0.578

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE12 | 0.58 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F12HA | 1.00 |
| F12HB2 | 1.00 |
| F12HB3 | 1.00 |
| F12HD2 | 1.00 |
| F12HE1 | 1.00 |
| F12HE2 | 1.00 |
| F12HZ | 1.00 |
| F12H | 1.00 |
| F12HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE12 | HA | 1.00 | 0.023 | 1.00 | 0.06 |
| PHE12 | HB2 | 1.00 | 0.018 | 1.00 | 0.73 |
| PHE12 | HB3 | 1.00 | 0.022 | 1.00 | 0.17 |
| PHE12 | HD1 | 1.00 | 0.002 | 1.00 | 8.62 |
| PHE12 | HD2 | 1.00 | 0.002 | 1.00 | 8.62 |
| PHE12 | HE1 | 1.00 | 0.039 | 0.10 | 0.00 |
| PHE12 | HE2 | 1.00 | 0.039 | 0.10 | 0.00 |
| PHE12 | HZ | 1.00 | 0.086 | 0.00 | 0.00 |
| PHE12 | H | 1.00 | 0.576 | 0.00 | 0.00 |

3.12.4 Detailed Probabilities of PHE12CD2:

Overall probability: 0.579

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE12 | 0.58 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F12HA | 1.00 |
| F12HB2 | 1.00 |
| F12HB3 | 1.00 |
| F12HD1 | 1.00 |
| F12HE1 | 1.00 |
| F12HE2 | 1.00 |
| F12HZ | 1.00 |
| F12H | 0.99 |
| F12HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE12 | HA | 1.00 | 0.023 | 1.00 | 0.06 |
| PHE12 | HB2 | 1.00 | 0.018 | 1.00 | 0.73 |
| PHE12 | HB3 | 1.00 | 0.022 | 1.00 | 0.17 |
| PHE12 | HD1 | 1.00 | 0.002 | 1.00 | 8.62 |
| PHE12 | HD2 | 1.00 | 0.002 | 1.00 | 8.62 |
| PHE12 | HE1 | 1.00 | 0.039 | 0.10 | 0.00 |
| PHE12 | HE2 | 1.00 | 0.039 | 0.10 | 0.00 |
| PHE12 | HZ | 1.00 | 0.086 | 0.00 | 0.00 |
| PHE12 | H | 0.99 | 0.576 | 0.01 | 0.00 |

3.12.5 Detailed Probabilities of PHE12CE1:

Overall probability: 0.567

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE12 | 0.57 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F12HD1 | 1.00 |
| F12HD2 | 1.00 |
| F12HE2 | 1.00 |
| F12HZ | 1.00 |
| F12HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE12 | HD1 | 1.00 | 0.046 | 0.00 | 0.00 |
| PHE12 | HD2 | 1.00 | 0.046 | 0.00 | 0.00 |
| PHE12 | HE1 | 1.00 | 0.004 | 1.00 | 8.35 |
| PHE12 | HE2 | 1.00 | 0.004 | 1.00 | 8.35 |
| PHE12 | HZ | 1.00 | 0.036 | 0.40 | 0.00 |
| PHE12 | HB2 | 0.90 | 0.001 | 1.00 | 0.80 |

3.12.6 Detailed Probabilities of PHE12CE2:

Overall probability: 0.486

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE12 | 0.49 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F12HB2 | 1.00 |
| F12HB3 | 1.00 |
| F12HD1 | 1.00 |
| F12HD2 | 1.00 |
| F12HE1 | 1.00 |
| F12HZ | 1.00 |
| F12HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE12 | HB2 | 1.00 | 0.001 | 1.00 | 0.80 |
| PHE12 | HB3 | 1.00 | 1.010 | 0.00 | 0.00 |
| PHE12 | HD1 | 1.00 | 0.046 | 0.00 | 0.00 |
| PHE12 | HD2 | 1.00 | 0.046 | 0.00 | 0.00 |
| PHE12 | HE1 | 1.00 | 0.004 | 1.00 | 8.35 |
| PHE12 | HE2 | 1.00 | 0.004 | 1.00 | 8.35 |
| PHE12 | HZ | 1.00 | 0.036 | 0.40 | 0.00 |

3.12.7 Detailed Probabilities of PHE12CZ:

Overall probability: 0.400

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE12 | 0.40 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F12HD1 | 1.00 |
| F12HD2 | 1.00 |
| F12HE1 | 1.00 |
| F12HE2 | 1.00 |
| F12HZ | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE12 | HD1 | 1.00 | 0.015 | 1.00 | 0.16 |
| PHE12 | HD2 | 1.00 | 0.015 | 1.00 | 0.16 |
| PHE12 | HE1 | 1.00 | 0.057 | 0.00 | 0.00 |
| PHE12 | HE2 | 1.00 | 0.057 | 0.00 | 0.00 |
| PHE12 | HZ | 1.00 | 0.104 | 0.00 | 0.00 |

3.12.8 Detailed Probabilities of PHE12N:

Overall probability: 0.389

Overall confidence: 0.929

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET11 | 0.60 | 0.83 |
| PHE12 | 0.34 | 1.00 |
| ILE13 | 0.02 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M11H | 1.00 |
| M11HG3 | 0.97 |
| M11HG2 | 0.98 |
| M11HB2 | 1.00 |
| M11HA | 1.00 |
| M11HB3 | 1.00 |
| F12HA | 1.00 |
| F12HB2 | 1.00 |
| F12HB3 | 1.00 |
| F12HD1 | 1.00 |
| F12HD2 | 0.99 |
| F12H | 1.00 |
| I13HA | 0.96 |
| I13H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET11 | HA | 1.00 | 0.004 | 1.00 | -263429.00 |
| MET11 | HB2 | 1.00 | 0.409 | 0.00 | 0.00 |
| MET11 | HB3 | 1.00 | 0.523 | 0.00 | 0.00 |
| MET11 | HG2 | 0.98 | 0.007 | 1.00 | -81657.00 |
| MET11 | HG3 | 0.97 | 0.002 | 1.00 | -81657.00 |
| PHE12 | HA | 1.00 | 0.164 | 0.00 | 0.00 |
| PHE12 | HB2 | 1.00 | 0.048 | 0.00 | 0.00 |
| PHE12 | HB3 | 1.00 | 0.001 | 1.00 | -101187.00 |
| PHE12 | HD1 | 1.00 | 1.267 | 0.00 | 0.00 |
| PHE12 | HD2 | 0.99 | 1.267 | 0.01 | 0.00 |
| PHE12 | H | 1.00 | 0.003 | 1.00 | -221406.00 |
| ILE13 | HA | 0.96 | 0.102 | 0.04 | 0.00 |
| ILE13 | H | 1.00 | 0.504 | 0.00 | 0.00 |

3.12.9 Detailed Probabilities of PHE12HA:

Overall probability: 0.733

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET11 | 1.00 | 0.50 |
| PHE12 | 0.63 | 1.00 |
| ILE13 | 0.75 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M11HA | 1.00 |
| M11H | 0.96 |
| F12HB2 | 1.00 |
| F12HB3 | 1.00 |
| F12HD1 | 1.00 |
| F12HD2 | 1.00 |
| F12H | 1.00 |
| F12HA | 1.00 |
| I13H | 1.00 |
| I13HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET11 | HA | 1.00 | 0.013 | 1.00 | 0.06 |
| MET11 | HB3 | 0.85 | 0.019 | 1.00 | 0.67 |
| PHE12 | HA | 1.00 | 0.077 | 0.00 | 0.00 |
| PHE12 | HB2 | 1.00 | 0.032 | 0.80 | 0.00 |
| PHE12 | HB3 | 1.00 | 0.006 | 1.00 | 0.46 |
| PHE12 | HD1 | 1.00 | 0.023 | 1.00 | 0.06 |
| PHE12 | HD2 | 1.00 | 0.023 | 1.00 | 0.06 |
| PHE12 | H | 1.00 | 0.164 | 0.00 | 0.00 |
| ILE13 | HA | 1.00 | 0.063 | 0.00 | 0.00 |
| ILE13 | H | 1.00 | 0.010 | 1.00 | -658236.00 |
| ILE13 | HG12 | 0.53 | 0.004 | 1.00 | 0.09 |
| ILE13 | HG13 | 0.66 | 0.002 | 1.00 | 0.07 |

3.12.10 Detailed Probabilities of PHE12HB2:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE12 | 0.88 | 1.00 |
| ILE13 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F12HA | 1.00 |
| F12HB3 | 1.00 |
| F12HD1 | 1.00 |
| F12HD2 | 1.00 |
| F12HE2 | 1.00 |
| F12H | 1.00 |
| F12HB2 | 1.00 |
| I13H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE12 | HA | 1.00 | 0.012 | 1.00 | 0.68 |
| PHE12 | HB2 | 1.00 | 0.004 | 1.00 | 6.62 |
| PHE12 | HB3 | 1.00 | 0.028 | 1.00 | 4.41 |
| PHE12 | HD1 | 1.00 | 0.018 | 1.00 | 0.73 |
| PHE12 | HD2 | 1.00 | 0.018 | 1.00 | 0.73 |
| PHE12 | HE2 | 1.00 | 0.001 | 1.00 | 0.80 |
| PHE12 | H | 1.00 | 0.048 | 0.00 | 0.00 |
| PHE12 | HE1 | 0.90 | 0.001 | 1.00 | 0.80 |
| ILE13 | H | 1.00 | 0.015 | 1.00 | -178480.00 |

3.12.11 Detailed Probabilities of PHE12HB3:

Overall probability: 0.663

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE12 | 0.64 | 1.00 |
| ILE13 | 0.80 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F12HA | 1.00 |
| F12HB2 | 1.00 |
| F12HD1 | 1.00 |
| F12HD2 | 1.00 |
| F12HE2 | 1.00 |
| F12H | 1.00 |
| F12HB3 | 1.00 |
| I13H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE12 | HA | 1.00 | 0.035 | 0.50 | 0.00 |
| PHE12 | HB2 | 1.00 | 0.043 | 0.00 | 0.00 |
| PHE12 | HB3 | 1.00 | 0.019 | 1.00 | 4.41 |
| PHE12 | HD1 | 1.00 | 0.022 | 1.00 | 0.17 |
| PHE12 | HD2 | 1.00 | 0.022 | 1.00 | 0.17 |
| PHE12 | HE2 | 1.00 | 1.010 | 0.00 | 0.00 |
| PHE12 | H | 1.00 | 0.001 | 1.00 | -101187.00 |
| ILE13 | H | 1.00 | 0.032 | 0.80 | 0.00 |

3.12.12 Detailed Probabilities of PHE12HD1:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE12 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F12HA | 1.00 |
| F12HB2 | 1.00 |
| F12HB3 | 1.00 |
| F12HD2 | 1.00 |
| F12HE1 | 1.00 |
| F12HE2 | 1.00 |
| F12HZ | 1.00 |
| F12H | 1.00 |
| F12HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE12 | HA | 1.00 | 0.017 | 1.00 | 0.27 |
| PHE12 | HB2 | 1.00 | 0.000 | 1.00 | 0.48 |
| PHE12 | HB3 | 1.00 | 0.000 | 1.00 | 0.49 |
| PHE12 | HD1 | 1.00 | 0.002 | 1.00 | 8.62 |
| PHE12 | HD2 | 1.00 | 0.002 | 1.00 | 8.62 |
| PHE12 | HE1 | 1.00 | 0.046 | 0.00 | 0.00 |
| PHE12 | HE2 | 1.00 | 0.046 | 0.00 | 0.00 |
| PHE12 | HZ | 1.00 | 0.015 | 1.00 | 0.16 |
| PHE12 | H | 1.00 | 1.267 | 0.00 | 0.00 |

3.12.13 Detailed Probabilities of PHE12HD2:

Overall probability: 0.668

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE12 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F12HA | 1.00 |
| F12HB2 | 1.00 |
| F12HB3 | 1.00 |
| F12HD1 | 1.00 |
| F12HE1 | 1.00 |
| F12HE2 | 1.00 |
| F12HZ | 1.00 |
| F12H | 0.99 |
| F12HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE12 | HA | 1.00 | 0.017 | 1.00 | 0.27 |
| PHE12 | HB2 | 1.00 | 0.000 | 1.00 | 0.48 |
| PHE12 | HB3 | 1.00 | 0.000 | 1.00 | 0.49 |
| PHE12 | HD1 | 1.00 | 0.002 | 1.00 | 8.62 |
| PHE12 | HD2 | 1.00 | 0.002 | 1.00 | 8.62 |
| PHE12 | HE1 | 1.00 | 0.046 | 0.00 | 0.00 |
| PHE12 | HE2 | 1.00 | 0.046 | 0.00 | 0.00 |
| PHE12 | HZ | 1.00 | 0.015 | 1.00 | 0.16 |
| PHE12 | H | 0.99 | 1.267 | 0.01 | 0.00 |

3.12.14 Detailed Probabilities of PHE12HE1:

Overall probability: 0.533

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE12 | 0.53 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F12HD1 | 1.00 |
| F12HD2 | 1.00 |
| F12HE2 | 1.00 |
| F12HZ | 1.00 |
| F12HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE12 | HD1 | 1.00 | 0.039 | 0.10 | 0.00 |
| PHE12 | HD2 | 1.00 | 0.039 | 0.10 | 0.00 |
| PHE12 | HE1 | 1.00 | 0.004 | 1.00 | 8.35 |
| PHE12 | HE2 | 1.00 | 0.004 | 1.00 | 8.35 |
| PHE12 | HZ | 1.00 | 0.057 | 0.00 | 0.00 |
| PHE12 | HA | 0.74 | 0.025 | 1.00 | 0.30 |

3.12.15 Detailed Probabilities of PHE12HE2:

Overall probability: 0.315

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE12 | 0.31 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F12HB2 | 1.00 |
| F12HB3 | 1.00 |
| F12HD1 | 1.00 |
| F12HD2 | 1.00 |
| F12HE1 | 1.00 |
| F12HZ | 1.00 |
| F12HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE12 | HB2 | 1.00 | 0.042 | 0.00 | 0.00 |
| PHE12 | HB3 | 1.00 | 0.042 | 0.00 | 0.00 |
| PHE12 | HD1 | 1.00 | 0.039 | 0.10 | 0.00 |
| PHE12 | HD2 | 1.00 | 0.039 | 0.10 | 0.00 |
| PHE12 | HE1 | 1.00 | 0.004 | 1.00 | 8.35 |
| PHE12 | HE2 | 1.00 | 0.004 | 1.00 | 8.35 |
| PHE12 | HZ | 1.00 | 0.057 | 0.00 | 0.00 |

3.12.16 Detailed Probabilities of PHE12HZ:

Overall probability: 0.160

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE12 | 0.16 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F12HD1 | 1.00 |
| F12HD2 | 1.00 |
| F12HE1 | 1.00 |
| F12HE2 | 1.00 |
| F12HZ | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE12 | HD1 | 1.00 | 0.086 | 0.00 | 0.00 |
| PHE12 | HD2 | 1.00 | 0.086 | 0.00 | 0.00 |
| PHE12 | HE1 | 1.00 | 0.036 | 0.40 | 0.00 |
| PHE12 | HE2 | 1.00 | 0.036 | 0.40 | 0.00 |
| PHE12 | HZ | 1.00 | 0.104 | 0.00 | 0.00 |

3.12.17 Detailed Probabilities of PHE12H:

Overall probability: 0.543

Overall confidence: 0.929

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET11 | 0.80 | 0.83 |
| PHE12 | 0.50 | 1.00 |
| I13 | 0.02 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M11H | 1.00 |
| M11HG3 | 0.97 |
| M11HG2 | 0.98 |
| M11HB2 | 1.00 |
| M11HA | 1.00 |
| M11HB3 | 1.00 |
| F12HA | 1.00 |
| F12HB2 | 1.00 |
| F12HB3 | 1.00 |
| F12HD1 | 1.00 |
| F12HD2 | 0.99 |
| F12H | 1.00 |
| I13HA | 0.96 |
| I13H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET11 | HA | 1.00 | 0.002 | 1.00 | 0.41 |
| MET11 | HB2 | 1.00 | 0.012 | 1.00 | 0.09 |
| MET11 | HB3 | 1.00 | 0.092 | 0.00 | 0.00 |
| MET11 | HG2 | 0.98 | 0.012 | 1.00 | 0.06 |
| MET11 | HG3 | 0.97 | 0.012 | 1.00 | 0.06 |
| PHE12 | HA | 1.00 | 0.114 | 0.00 | 0.00 |
| PHE12 | HB2 | 1.00 | 0.005 | 1.00 | 0.11 |
| PHE12 | HB3 | 1.00 | 0.004 | 1.00 | 0.09 |
| PHE12 | HD1 | 1.00 | 0.576 | 0.00 | 0.00 |
| PHE12 | HD2 | 0.99 | 0.576 | 0.01 | 0.00 |
| PHE12 | H | 1.00 | 0.003 | 1.00 | -221406.00 |
| I13 | HA | 0.96 | 0.341 | 0.04 | 0.00 |
| I13 | H | 1.00 | 0.505 | 0.00 | 0.00 |

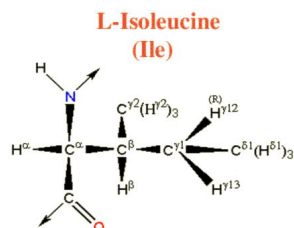
3.13 ILE(13)

Figure 3: Image from the BMRB

Residue probability: 0.927

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|--------------|-------------|---------|--------|---------------------|--------------------|
| C | 174.482 | 175.926 | 2.710 | 0.000 | 0.000 |
| CA 3.13.1 | 60.425 | 61.717 | 4.152 | 0.731 | 1.000 |
| CB 3.13.2 | 38.641 | 38.702 | 3.945 | 1.000 | 1.000 |
| CG1 3.13.3 | 28.205 | 27.785 | 2.037 | 1.000 | 1.000 |
| CG2 3.13.4 | 17.951 | 17.574 | 1.928 | 1.000 | 1.000 |
| CD1 3.13.5 | 14.943 | 13.545 | 3.646 | 1.000 | 1.000 |
| N 3.13.6 | 122.825 | 121.467 | 6.098 | 0.900 | 1.000 |
| HA 3.13.7 | 4.149 | 4.185 | 1.403 | 0.731 | 1.000 |
| HB 3.13.8 | 1.462 | 1.776 | 0.310 | 0.889 | 1.000 |
| HG12 3.13.9 | 1.491 | 1.271 | 0.411 | 0.875 | 1.000 |
| HG13 3.13.10 | 0.747 | 1.186 | 0.426 | 1.000 | 1.000 |
| HG2 3.13.11 | 0.764 | 0.762 | 0.283 | 1.000 | 1.000 |
| HD1 3.13.12 | 0.747 | 0.668 | 0.293 | 1.000 | 1.000 |
| H 3.13.13 | 7.950 | 8.301 | 0.685 | 0.923 | 1.000 |

3.13.1 Detailed Probabilities of ILE13CA:

Overall probability: 0.731

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE12 | 0.02 | 1.00 |
| ILE13 | 1.00 | 1.00 |
| GLN14 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| F12H | 0.96 |
| F12HA | 1.00 |
| I13HB | 1.00 |
| I13HG12 | 1.00 |
| I13HG13 | 1.00 |
| I13HG21 | 1.00 |
| I13HD11 | 0.97 |
| I13H | 1.00 |
| I13HA | 1.00 |
| Q14H | 1.00 |
| Q14HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE12 | HA | 1.00 | 0.063 | 0.00 | 0.00 |
| PHE12 | H | 0.96 | 0.341 | 0.04 | 0.00 |
| ILE13 | HA | 1.00 | 0.005 | 1.00 | 14.00 |
| ILE13 | HB | 1.00 | 0.006 | 1.00 | 0.73 |
| ILE13 | HG12 | 1.00 | 0.023 | 1.00 | 0.73 |
| ILE13 | HG13 | 1.00 | 0.008 | 1.00 | 1.02 |
| ILE13 | HG21 | 1.00 | 0.009 | 1.00 | 1.02 |
| ILE13 | HD11 | 0.97 | 0.008 | 1.00 | 1.02 |
| ILE13 | H | 1.00 | 0.016 | 1.00 | 0.86 |
| GLN14 | HA | 1.00 | 0.063 | 0.00 | 0.00 |
| GLN14 | H | 1.00 | 0.009 | 1.00 | 0.86 |

3.13.2 Detailed Probabilities of ILE13CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE13 | 1.00 | 1.00 |
| GLN14 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I13HA | 1.00 |
| I13HG12 | 1.00 |
| I13HG13 | 1.00 |
| I13HG21 | 1.00 |
| I13HD11 | 1.00 |
| I13H | 1.00 |
| I13HB | 1.00 |
| Q14H | 1.00 |

NOESY contacts detailed probability

3.13 ILE(13)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE13 | HA | 1.00 | 0.004 | 1.00 | 0.23 |
| ILE13 | HB | 1.00 | 0.001 | 1.00 | 4.70 |
| ILE13 | HG12 | 1.00 | 0.028 | 1.00 | 4.70 |
| ILE13 | HG13 | 1.00 | 0.007 | 1.00 | 2.30 |
| ILE13 | HG21 | 1.00 | 0.010 | 1.00 | 2.30 |
| ILE13 | HD11 | 1.00 | 0.007 | 1.00 | 2.30 |
| ILE13 | H | 1.00 | 0.004 | 1.00 | 0.51 |
| GLN14 | H | 1.00 | 0.021 | 1.00 | 0.51 |

3.13.3 Detailed Probabilities of ILE13CG1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE13 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I13HA | 1.00 |
| I13HB | 1.00 |
| I13HG12 | 1.00 |
| I13HG21 | 1.00 |
| I13HD11 | 1.00 |
| I13H | 1.00 |
| I13HG13 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE13 | HA | 1.00 | 0.003 | 1.00 | 0.26 |
| ILE13 | HB | 1.00 | 0.025 | 1.00 | 1.96 |
| ILE13 | HG12 | 1.00 | 0.004 | 1.00 | 1.96 |
| ILE13 | HG13 | 1.00 | 0.003 | 1.00 | 5.18 |
| ILE13 | HG21 | 1.00 | 0.014 | 1.00 | 5.18 |
| ILE13 | HD11 | 1.00 | 0.003 | 1.00 | 5.18 |
| ILE13 | H | 1.00 | 0.005 | 1.00 | 0.21 |

3.13.4 Detailed Probabilities of ILE13CG2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE13 | 1.00 | 1.00 |
| GLN14 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I13HA | 1.00 |
| I13HB | 1.00 |
| I13HG12 | 1.00 |
| I13HG13 | 1.00 |
| I13HG22 | 1.00 |
| I13HD11 | 0.99 |
| I13H | 1.00 |
| Q14H | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE13 | HA | 1.00 | 0.008 | 1.00 | 0.76 |
| ILE13 | HB | 1.00 | 0.005 | 1.00 | 1.72 |
| ILE13 | HG12 | 1.00 | 0.024 | 1.00 | 1.72 |
| ILE13 | HG13 | 1.00 | 0.013 | 1.00 | 35.39 |
| ILE13 | HG21 | 1.00 | 0.004 | 1.00 | 35.39 |
| ILE13 | HD11 | 0.99 | 0.013 | 1.00 | 35.39 |
| ILE13 | H | 1.00 | 0.014 | 1.00 | 0.68 |
| GLN14 | H | 0.99 | 0.011 | 1.00 | 0.68 |

3.13.5 Detailed Probabilities of ILE13CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE13 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I13HA | 0.97 |
| I13HB | 1.00 |
| I13HG12 | 1.00 |
| I13HG13 | 1.00 |
| I13HG21 | 0.99 |
| I13HD12 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE13 | HA | 0.97 | 0.011 | 1.00 | 0.33 |
| ILE13 | HB | 1.00 | 0.020 | 1.00 | 2.27 |
| ILE13 | HG12 | 1.00 | 0.009 | 1.00 | 2.27 |
| ILE13 | HG13 | 1.00 | 0.019 | 1.00 | 40.86 |
| ILE13 | HG21 | 0.99 | 0.002 | 1.00 | 40.86 |
| ILE13 | HD11 | 1.00 | 0.019 | 1.00 | 40.86 |
| ILE13 | H | 0.94 | 0.003 | 1.00 | 0.34 |

3.13.6 Detailed Probabilities of ILE13N:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE12 | 0.70 | 1.00 |
| ILE13 | 1.00 | 1.00 |
| GLN14 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| F12HB3 | 1.00 |
| F12HA | 1.00 |
| F12HB2 | 1.00 |
| F12H | 1.00 |
| I13HA | 1.00 |
| I13HB | 1.00 |
| I13HG12 | 1.00 |
| I13HG13 | 1.00 |
| I13HG21 | 1.00 |
| I13H | 1.00 |
| Q14H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE12 | HA | 1.00 | 0.010 | 1.00 | -658236.00 |
| PHE12 | HB2 | 1.00 | 0.015 | 1.00 | -178480.00 |
| PHE12 | HB3 | 1.00 | 0.032 | 0.80 | 0.00 |
| PHE12 | H | 1.00 | 0.505 | 0.00 | 0.00 |
| ILE13 | HA | 1.00 | 0.003 | 1.00 | -164709.00 |
| ILE13 | HB | 1.00 | 0.004 | 1.00 | -693226.00 |
| ILE13 | HG12 | 1.00 | 0.025 | 1.00 | -693226.00 |
| ILE13 | HG13 | 1.00 | 0.004 | 1.00 | -507972.00 |
| ILE13 | HG21 | 1.00 | 0.013 | 1.00 | -507972.00 |
| ILE13 | H | 1.00 | 0.004 | 1.00 | -2221981.00 |
| ILE13 | HD11 | 0.94 | 0.004 | 1.00 | -507972.00 |
| GLN14 | H | 1.00 | 0.021 | 1.00 | -2221981.00 |

3.13.7 Detailed Probabilities of ILE13HA:

Overall probability: 0.731

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE12 | 0.02 | 1.00 |
| ILE13 | 1.00 | 1.00 |
| GLN14 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| F12H | 0.96 |
| F12HA | 1.00 |
| I13HB | 1.00 |
| I13HG12 | 1.00 |
| I13HG13 | 1.00 |
| I13HG21 | 1.00 |
| I13HD11 | 0.97 |
| I13H | 1.00 |
| I13HA | 1.00 |
| Q14H | 1.00 |
| Q14HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE12 | HA | 1.00 | 0.040 | 0.00 | 0.00 |
| PHE12 | H | 0.96 | 0.102 | 0.04 | 0.00 |
| ILE13 | HA | 1.00 | 0.005 | 1.00 | 14.00 |
| ILE13 | HB | 1.00 | 0.004 | 1.00 | 0.23 |
| ILE13 | HG12 | 1.00 | 0.003 | 1.00 | 0.20 |
| ILE13 | HG13 | 1.00 | 0.003 | 1.00 | 0.26 |
| ILE13 | HG21 | 1.00 | 0.008 | 1.00 | 0.76 |
| ILE13 | HD11 | 0.97 | 0.011 | 1.00 | 0.33 |
| ILE13 | H | 1.00 | 0.003 | 1.00 | -164709.00 |
| GLN14 | HA | 1.00 | 0.059 | 0.00 | 0.00 |
| GLN14 | H | 1.00 | 0.003 | 1.00 | -1378659.00 |

3.13.8 Detailed Probabilities of ILE13HB:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE13 | 0.86 | 1.00 |
| GLN14 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I13HA | 1.00 |
| I13HG12 | 1.00 |
| I13HG13 | 1.00 |
| I13HG21 | 1.00 |
| I13HD11 | 1.00 |
| I13H | 1.00 |
| I13HB | 1.00 |
| Q14H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE13 | HA | 1.00 | 0.006 | 1.00 | 0.73 |
| ILE13 | HB | 1.00 | 0.001 | 1.00 | 4.70 |
| ILE13 | HG12 | 1.00 | 0.545 | 0.00 | 0.00 |
| ILE13 | HG13 | 1.00 | 0.025 | 1.00 | 1.96 |
| ILE13 | HG21 | 1.00 | 0.005 | 1.00 | 1.72 |
| ILE13 | HD11 | 1.00 | 0.020 | 1.00 | 2.27 |
| ILE13 | H | 1.00 | 0.004 | 1.00 | -693226.00 |
| GLN14 | H | 1.00 | 0.005 | 1.00 | -169959.00 |
| GLN14 | HA | 0.89 | 0.000 | 1.00 | 0.27 |

3.13.9 Detailed Probabilities of ILE13HG12:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE13 | 0.86 | 1.00 |
| GLN14 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I13HA | 1.00 |
| I13HB | 1.00 |
| I13HG13 | 1.00 |
| I13HG21 | 1.00 |
| I13HD11 | 1.00 |
| I13H | 1.00 |
| I13HG12 | 1.00 |
| Q14H | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE13 | HA | 1.00 | 0.023 | 1.00 | 0.73 |
| ILE13 | HB | 1.00 | 0.028 | 1.00 | 4.70 |
| ILE13 | HG12 | 1.00 | 0.516 | 0.00 | 0.00 |
| ILE13 | HG13 | 1.00 | 0.004 | 1.00 | 1.96 |
| ILE13 | HG21 | 1.00 | 0.024 | 1.00 | 1.72 |
| ILE13 | HD11 | 1.00 | 0.009 | 1.00 | 2.27 |
| ILE13 | H | 1.00 | 0.025 | 1.00 | -693226.00 |
| GLN14 | H | 0.99 | 0.024 | 1.00 | -169959.00 |

3.13.10 Detailed Probabilities of ILE13HG13:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE13 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I13HA | 1.00 |
| I13HB | 1.00 |
| I13HG12 | 1.00 |
| I13HG21 | 1.00 |
| I13HD11 | 1.00 |
| I13H | 1.00 |
| I13HG13 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE13 | HA | 1.00 | 0.008 | 1.00 | 1.02 |
| ILE13 | HB | 1.00 | 0.007 | 1.00 | 2.30 |
| ILE13 | HG12 | 1.00 | 0.002 | 1.00 | 3.66 |
| ILE13 | HG13 | 1.00 | 0.003 | 1.00 | 5.18 |
| ILE13 | HG21 | 1.00 | 0.013 | 1.00 | 35.39 |
| ILE13 | HD11 | 1.00 | 0.019 | 1.00 | 40.86 |
| ILE13 | H | 1.00 | 0.004 | 1.00 | -507972.00 |

3.13.11 Detailed Probabilities of ILE13HG21:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE13 | 1.00 | 1.00 |
| GLN14 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I13HA | 1.00 |
| I13HB | 1.00 |
| I13HG12 | 1.00 |
| I13HG13 | 1.00 |
| I13HG22 | 1.00 |
| I13HD11 | 0.99 |
| I13H | 1.00 |
| Q14H | 0.99 |

NOESY contacts detailed probability

3.13 ILE(13)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE13 | HA | 1.00 | 0.009 | 1.00 | 1.02 |
| ILE13 | HB | 1.00 | 0.010 | 1.00 | 2.30 |
| ILE13 | HG12 | 1.00 | 0.015 | 1.00 | 3.66 |
| ILE13 | HG13 | 1.00 | 0.014 | 1.00 | 5.18 |
| ILE13 | HG21 | 1.00 | 0.004 | 1.00 | 35.39 |
| ILE13 | HD11 | 0.99 | 0.002 | 1.00 | 40.86 |
| ILE13 | H | 1.00 | 0.013 | 1.00 | -507972.00 |
| GLN14 | H | 0.99 | 0.008 | 1.00 | -866555.00 |
| GLN14 | HA | 0.69 | 0.002 | 1.00 | 0.21 |

3.13.12 Detailed Probabilities of ILE13HD11:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE13 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I13HA | 0.97 |
| I13HB | 1.00 |
| I13HG12 | 1.00 |
| I13HG13 | 1.00 |
| I13HG21 | 0.99 |
| I13HD12 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE13 | HA | 0.97 | 0.008 | 1.00 | 1.02 |
| ILE13 | HB | 1.00 | 0.007 | 1.00 | 2.30 |
| ILE13 | HG12 | 1.00 | 0.002 | 1.00 | 3.66 |
| ILE13 | HG13 | 1.00 | 0.003 | 1.00 | 5.18 |
| ILE13 | HG21 | 0.99 | 0.013 | 1.00 | 35.39 |
| ILE13 | HD11 | 1.00 | 0.019 | 1.00 | 40.86 |
| ILE13 | H | 0.94 | 0.004 | 1.00 | -507972.00 |

3.13.13 Detailed Probabilities of ILE13H:

Overall probability: 0.923

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE12 | 0.75 | 1.00 |
| ILE13 | 1.00 | 1.00 |
| GLN14 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| F12HB3 | 1.00 |
| F12HA | 1.00 |
| F12HB2 | 1.00 |
| F12H | 1.00 |
| I13HA | 1.00 |
| I13HB | 1.00 |
| I13HG12 | 1.00 |
| I13HG13 | 1.00 |
| I13HG21 | 1.00 |
| I13H | 1.00 |
| Q14H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE12 | HA | 1.00 | 0.006 | 1.00 | 0.95 |
| PHE12 | HB2 | 1.00 | 0.001 | 1.00 | 0.10 |
| PHE12 | HB3 | 1.00 | 0.013 | 1.00 | 0.10 |
| PHE12 | H | 1.00 | 0.504 | 0.00 | 0.00 |
| ILE13 | HA | 1.00 | 0.016 | 1.00 | 0.86 |
| ILE13 | HB | 1.00 | 0.004 | 1.00 | 0.51 |
| ILE13 | HG12 | 1.00 | 0.006 | 1.00 | 0.26 |
| ILE13 | HG13 | 1.00 | 0.005 | 1.00 | 0.21 |
| ILE13 | HG21 | 1.00 | 0.014 | 1.00 | 0.68 |
| ILE13 | H | 1.00 | 0.004 | 1.00 | -2221981.00 |
| ILE13 | HD11 | 0.94 | 0.003 | 1.00 | 0.34 |
| GLN14 | H | 1.00 | 0.021 | 1.00 | -4138682.00 |
| GLN14 | HB2 | 0.56 | 0.024 | 1.00 | 0.30 |

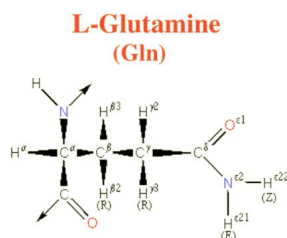
3.14 GLN(14)

Figure 4: Image from the BMRB

Residue probability: 0.854

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|--------------|-------------|---------|--------|---------------------|--------------------|
| C | 175.002 | 176.405 | 1.998 | 0.000 | 0.000 |
| CA 3.14.1 | 54.860 | 56.667 | 2.318 | 0.833 | 1.000 |
| CB 3.14.2 | 31.276 | 29.436 | 2.799 | 0.667 | 1.000 |
| CG 3.14.3 | 33.871 | 33.781 | 1.871 | 1.000 | 1.000 |
| N 3.14.4 | 125.864 | 119.799 | 3.762 | 1.000 | 1.000 |
| NE2 3.14.5 | 111.842 | 111.924 | 2.434 | 1.000 | 1.000 |
| HA 3.14.6 | 4.587 | 4.265 | 0.455 | 0.800 | 1.000 |
| HB2 3.14.7 | 2.149 | 2.047 | 0.290 | 0.889 | 1.000 |
| HB3 3.14.8 | 1.926 | 2.012 | 0.313 | 1.000 | 1.000 |
| HG2 3.14.9 | 2.276 | 2.308 | 0.289 | 1.000 | 1.000 |
| HG3 3.14.10 | 2.370 | 2.284 | 0.313 | 0.778 | 1.000 |
| H 3.14.11 | 7.925 | 8.232 | 0.711 | 0.923 | 1.000 |
| HE21 3.14.12 | 7.513 | 7.217 | 0.496 | 0.714 | 1.000 |
| HE22 3.14.13 | 6.854 | 7.041 | 0.463 | 0.500 | 1.000 |

3.14.1 Detailed Probabilities of GLN14CA:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE13 | 0.67 | 1.00 |
| GLN14 | 0.86 | 1.00 |
| THR15 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| I13HA | 1.00 |
| Q14HB2 | 1.00 |
| Q14HB3 | 1.00 |
| Q14HG2 | 1.00 |
| Q14HG3 | 1.00 |
| Q14H | 1.00 |
| Q14HA | 1.00 |
| T15HA | 1.00 |
| T15H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE13 | HA | 1.00 | 0.059 | 0.00 | 0.00 |
| ILE13 | HB | 0.89 | 0.000 | 1.00 | 0.27 |
| ILE13 | HG21 | 0.70 | 0.002 | 1.00 | 0.21 |
| GLN14 | HA | 1.00 | 0.023 | 1.00 | 10.54 |
| GLN14 | HB2 | 1.00 | 0.002 | 1.00 | 0.78 |
| GLN14 | HB3 | 1.00 | 0.005 | 1.00 | 0.41 |
| GLN14 | HG2 | 1.00 | 0.009 | 1.00 | 0.44 |
| GLN14 | HG3 | 1.00 | 0.008 | 1.00 | 0.28 |
| GLN14 | H | 1.00 | 0.161 | 0.00 | 0.00 |
| GLN14 | HE21 | 0.94 | 0.020 | 1.00 | 0.16 |
| THR15 | HA | 1.00 | 0.024 | 1.00 | 0.13 |
| THR15 | H | 1.00 | 0.005 | 1.00 | 1.18 |

3.14.2 Detailed Probabilities of GLN14CB:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN14 | 0.63 | 1.00 |
| THR15 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q14HA | 1.00 |
| Q14HB3 | 1.00 |
| Q14HG2 | 1.00 |
| Q14HG3 | 1.00 |
| Q14H | 1.00 |
| Q14HE21 | 1.00 |
| Q14HE22 | 1.00 |
| Q14HB2 | 1.00 |
| T15H | 1.00 |

NOESY contacts detailed probability

3.14 GLN(14)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN14 | HA | 1.00 | 0.009 | 1.00 | 0.37 |
| GLN14 | HB2 | 1.00 | 0.001 | 1.00 | 28.97 |
| GLN14 | HB3 | 1.00 | 0.022 | 1.00 | 9.15 |
| GLN14 | HG2 | 1.00 | 0.017 | 1.00 | 3.78 |
| GLN14 | HG3 | 1.00 | 0.077 | 0.00 | 0.00 |
| GLN14 | H | 1.00 | 0.001 | 1.00 | 0.30 |
| GLN14 | HE21 | 1.00 | 0.123 | 0.00 | 0.00 |
| GLN14 | HE22 | 1.00 | 0.354 | 0.00 | 0.00 |
| THR15 | H | 1.00 | 0.012 | 1.00 | 0.40 |

3.14.3 Detailed Probabilities of GLN14CG:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN14 | 1.00 | 1.00 |
| THR15 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q14HA | 1.00 |
| Q14HB2 | 1.00 |
| Q14HB3 | 1.00 |
| Q14HG2 | 1.00 |
| Q14H | 1.00 |
| Q14HE21 | 1.00 |
| Q14HE22 | 1.00 |
| Q14HG3 | 1.00 |
| T15H | 0.95 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN14 | HA | 1.00 | 0.006 | 1.00 | 0.39 |
| GLN14 | HB2 | 1.00 | 0.005 | 1.00 | 1.56 |
| GLN14 | HB3 | 1.00 | 0.002 | 1.00 | 0.93 |
| GLN14 | HG2 | 1.00 | 0.005 | 1.00 | 9.65 |
| GLN14 | HG3 | 1.00 | 0.006 | 1.00 | 13.54 |
| GLN14 | H | 1.00 | 0.002 | 1.00 | 0.23 |
| GLN14 | HE21 | 1.00 | 0.007 | 1.00 | 0.16 |
| GLN14 | HE22 | 1.00 | 0.010 | 1.00 | 0.09 |
| THR15 | H | 0.95 | 0.000 | 1.00 | 0.12 |

3.14.4 Detailed Probabilities of GLN14N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE13 | 1.00 | 1.00 |
| GLN14 | 1.00 | 1.00 |
| THR15 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I13HG23 | 0.99 |
| I13HB | 1.00 |
| I13HG12 | 0.99 |
| I13H | 1.00 |
| I13HA | 1.00 |
| Q14HA | 1.00 |
| Q14HB2 | 1.00 |
| Q14HB3 | 1.00 |
| Q14HG2 | 1.00 |
| Q14HG3 | 1.00 |
| Q14H | 1.00 |
| T15H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE13 | HA | 1.00 | 0.003 | 1.00 | -1378659.00 |
| ILE13 | HB | 1.00 | 0.005 | 1.00 | -169959.00 |
| ILE13 | HG12 | 0.99 | 0.024 | 1.00 | -169959.00 |
| ILE13 | HG21 | 0.99 | 0.008 | 1.00 | -866555.00 |
| ILE13 | H | 1.00 | 0.021 | 1.00 | -4138682.00 |
| ILE13 | HG13 | 0.94 | 0.009 | 1.00 | -866555.00 |
| GLN14 | HA | 1.00 | 0.013 | 1.00 | -431341.00 |
| GLN14 | HB2 | 1.00 | 0.001 | 1.00 | -450009.00 |
| GLN14 | HB3 | 1.00 | 0.004 | 1.00 | -604321.00 |
| GLN14 | HG2 | 1.00 | 0.003 | 1.00 | -204963.00 |
| GLN14 | HG3 | 1.00 | 0.007 | 1.00 | -240778.00 |
| GLN14 | H | 1.00 | 0.004 | 1.00 | -4138682.00 |
| THR15 | H | 1.00 | 0.000 | 1.00 | -85708.00 |

3.14.5 Detailed Probabilities of GLN14NE2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN14 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q14HB2 | 1.00 |
| Q14HB3 | 1.00 |
| Q14HG2 | 1.00 |
| Q14HG3 | 1.00 |
| Q14HE22 | 1.00 |
| Q14HE21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN14 | HB2 | 1.00 | 0.008 | 1.00 | -131951.00 |
| GLN14 | HB3 | 1.00 | 0.004 | 1.00 | -129963.00 |
| GLN14 | HG2 | 1.00 | 0.000 | 1.00 | -447572.00 |
| GLN14 | HG3 | 1.00 | 0.007 | 1.00 | -597794.00 |
| GLN14 | HE21 | 1.00 | 0.003 | 1.00 | -22805602.00 |
| GLN14 | HE22 | 1.00 | 0.004 | 1.00 | -11763225.00 |
| GLN14 | HA | 0.94 | 0.021 | 1.00 | -106811.00 |

3.14.6 Detailed Probabilities of GLN14HA:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE13 | 0.00 | 1.00 |
| GLN14 | 1.00 | 1.00 |
| THR15 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| I13HA | 1.00 |
| Q14HB2 | 1.00 |
| Q14HB3 | 1.00 |
| Q14HG2 | 1.00 |
| Q14HG3 | 1.00 |
| Q14H | 1.00 |
| Q14HA | 1.00 |
| T15HA | 1.00 |
| T15H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE13 | HA | 1.00 | 0.063 | 0.00 | 0.00 |
| GLN14 | HA | 1.00 | 0.023 | 1.00 | 10.54 |
| GLN14 | HB2 | 1.00 | 0.009 | 1.00 | 0.37 |
| GLN14 | HB3 | 1.00 | 0.010 | 1.00 | 0.48 |
| GLN14 | HG2 | 1.00 | 0.006 | 1.00 | 0.45 |
| GLN14 | HG3 | 1.00 | 0.006 | 1.00 | 0.39 |
| GLN14 | H | 1.00 | 0.013 | 1.00 | -431341.00 |
| GLN14 | HE21 | 0.94 | 0.021 | 1.00 | -106811.00 |
| THR15 | HA | 1.00 | 0.237 | 0.00 | 0.00 |
| THR15 | H | 1.00 | 0.006 | 1.00 | -2463304.00 |

3.14.7 Detailed Probabilities of GLN14HB2:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN14 | 0.88 | 1.00 |
| THR15 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q14HA | 1.00 |
| Q14HB3 | 1.00 |
| Q14HG2 | 1.00 |
| Q14HG3 | 1.00 |
| Q14H | 1.00 |
| Q14HE21 | 1.00 |
| Q14HE22 | 1.00 |
| Q14HB2 | 1.00 |
| T15H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN14 | HA | 1.00 | 0.002 | 1.00 | 0.78 |
| GLN14 | HB2 | 1.00 | 0.001 | 1.00 | 28.97 |
| GLN14 | HB3 | 1.00 | 0.001 | 1.00 | 9.75 |
| GLN14 | HG2 | 1.00 | 0.011 | 1.00 | 1.38 |
| GLN14 | HG3 | 1.00 | 0.005 | 1.00 | 1.56 |
| GLN14 | H | 1.00 | 0.001 | 1.00 | -450009.00 |
| GLN14 | HE21 | 1.00 | 0.008 | 1.00 | -131951.00 |
| GLN14 | HE22 | 1.00 | 0.128 | 0.00 | 0.00 |
| THR15 | H | 1.00 | 0.001 | 1.00 | -771258.00 |

3.14.8 Detailed Probabilities of GLN14HB3:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN14 | 1.00 | 1.00 |
| THR15 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q14HA | 1.00 |
| Q14HB2 | 1.00 |
| Q14HG2 | 1.00 |
| Q14HG3 | 1.00 |
| Q14H | 1.00 |
| Q14HE21 | 1.00 |
| Q14HE22 | 1.00 |
| Q14HB3 | 1.00 |
| T15H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN14 | HA | 1.00 | 0.005 | 1.00 | 0.41 |
| GLN14 | HB2 | 1.00 | 0.022 | 1.00 | 9.15 |
| GLN14 | HB3 | 1.00 | 0.025 | 1.00 | 92.80 |
| GLN14 | HG2 | 1.00 | 0.003 | 1.00 | 0.86 |
| GLN14 | HG3 | 1.00 | 0.002 | 1.00 | 0.93 |
| GLN14 | H | 1.00 | 0.004 | 1.00 | -604321.00 |
| GLN14 | HE21 | 1.00 | 0.004 | 1.00 | -129963.00 |
| GLN14 | HE22 | 1.00 | 0.006 | 1.00 | -89935.00 |
| THR15 | H | 1.00 | 0.002 | 1.00 | -389406.00 |

3.14.9 Detailed Probabilities of GLN14HG2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN14 | 1.00 | 1.00 |
| THR15 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q14HA | 1.00 |
| Q14HB2 | 1.00 |
| Q14HB3 | 1.00 |
| Q14HG3 | 1.00 |
| Q14H | 1.00 |
| Q14HE21 | 1.00 |
| Q14HE22 | 1.00 |
| Q14HG2 | 1.00 |
| T15H | 0.97 |

NOESY contacts detailed probability

3.14 GLN(14)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN14 | HA | 1.00 | 0.009 | 1.00 | 0.44 |
| GLN14 | HB2 | 1.00 | 0.017 | 1.00 | 3.78 |
| GLN14 | HB3 | 1.00 | 0.027 | 1.00 | 1.72 |
| GLN14 | HG2 | 1.00 | 0.001 | 1.00 | 13.25 |
| GLN14 | HG3 | 1.00 | 0.005 | 1.00 | 9.65 |
| GLN14 | H | 1.00 | 0.003 | 1.00 | -204963.00 |
| GLN14 | HE21 | 1.00 | 0.000 | 1.00 | -447572.00 |
| GLN14 | HE22 | 1.00 | 0.001 | 1.00 | -229485.00 |
| THR15 | H | 0.97 | 0.008 | 1.00 | -257029.00 |

3.14.10 Detailed Probabilities of GLN14HG3:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN14 | 0.75 | 1.00 |
| THR15 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q14HA | 1.00 |
| Q14HB2 | 1.00 |
| Q14HB3 | 1.00 |
| Q14HG2 | 1.00 |
| Q14H | 1.00 |
| Q14HE21 | 1.00 |
| Q14HE22 | 1.00 |
| Q14HG3 | 1.00 |
| T15H | 0.95 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN14 | HA | 1.00 | 0.008 | 1.00 | 0.28 |
| GLN14 | HB2 | 1.00 | 0.077 | 0.00 | 0.00 |
| GLN14 | HB3 | 1.00 | 0.067 | 0.00 | 0.00 |
| GLN14 | HG2 | 1.00 | 0.006 | 1.00 | 9.54 |
| GLN14 | HG3 | 1.00 | 0.006 | 1.00 | 13.54 |
| GLN14 | H | 1.00 | 0.007 | 1.00 | -240778.00 |
| GLN14 | HE21 | 1.00 | 0.007 | 1.00 | -597794.00 |
| GLN14 | HE22 | 1.00 | 0.005 | 1.00 | -274148.00 |
| THR15 | H | 0.95 | 0.009 | 1.00 | -239767.00 |

3.14.11 Detailed Probabilities of GLN14H:

Overall probability: 0.923

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE13 | 1.00 | 1.00 |
| GLN14 | 0.83 | 1.00 |
| THR15 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I13HG23 | 0.99 |
| I13HB | 1.00 |
| I13HG12 | 0.99 |
| I13H | 1.00 |
| I13HA | 1.00 |
| Q14HA | 1.00 |
| Q14HB2 | 1.00 |
| Q14HB3 | 1.00 |
| Q14HG2 | 1.00 |
| Q14HG3 | 1.00 |
| Q14H | 1.00 |
| T15H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE13 | HA | 1.00 | 0.009 | 1.00 | 0.86 |
| ILE13 | HB | 1.00 | 0.021 | 1.00 | 0.51 |
| ILE13 | HG12 | 0.99 | 0.019 | 1.00 | 0.26 |
| ILE13 | HG21 | 0.99 | 0.011 | 1.00 | 0.68 |
| ILE13 | H | 1.00 | 0.021 | 1.00 | -2221981.00 |
| ILE13 | HG13 | 0.94 | 0.020 | 1.00 | 0.21 |
| GLN14 | HA | 1.00 | 0.161 | 0.00 | 0.00 |
| GLN14 | HB2 | 1.00 | 0.001 | 1.00 | 0.30 |
| GLN14 | HB3 | 1.00 | 0.009 | 1.00 | 0.37 |
| GLN14 | HG2 | 1.00 | 0.005 | 1.00 | 0.22 |
| GLN14 | HG3 | 1.00 | 0.002 | 1.00 | 0.23 |
| GLN14 | H | 1.00 | 0.004 | 1.00 | -4138682.00 |
| THR15 | H | 1.00 | 0.003 | 1.00 | -149157.00 |

3.14.12 Detailed Probabilities of GLN14HE21:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN14 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q14HB2 | 1.00 |
| Q14HB3 | 1.00 |
| Q14HG2 | 1.00 |
| Q14HG3 | 1.00 |
| Q14HE22 | 1.00 |
| Q14HE21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN14 | HB2 | 1.00 | 0.123 | 0.00 | 0.00 |
| GLN14 | HB3 | 1.00 | 0.301 | 0.00 | 0.00 |
| GLN14 | HG2 | 1.00 | 0.007 | 1.00 | 0.21 |
| GLN14 | HG3 | 1.00 | 0.007 | 1.00 | 0.16 |
| GLN14 | HE21 | 1.00 | 0.003 | 1.00 | -22805602.00 |
| GLN14 | HE22 | 1.00 | 0.002 | 1.00 | -10911006.00 |
| GLN14 | HA | 0.94 | 0.020 | 1.00 | 0.16 |

3.14.13 Detailed Probabilities of GLN14HE22:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN14 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q14HB2 | 1.00 |
| Q14HB3 | 1.00 |
| Q14HG2 | 1.00 |
| Q14HG3 | 1.00 |
| Q14HE21 | 1.00 |
| Q14HE22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN14 | HB2 | 1.00 | 0.354 | 0.00 | 0.00 |
| GLN14 | HB3 | 1.00 | 0.049 | 0.00 | 0.00 |
| GLN14 | HG2 | 1.00 | 0.652 | 0.00 | 0.00 |
| GLN14 | HG3 | 1.00 | 0.010 | 1.00 | 0.09 |
| GLN14 | HE21 | 1.00 | 0.004 | 1.00 | -11763225.00 |
| GLN14 | HE22 | 1.00 | 0.003 | 1.00 | -25132448.00 |

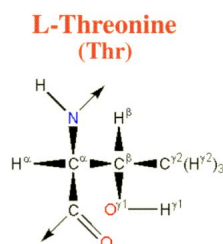
3.15 THR(15)

Figure 5: Image from the BMRB

Residue probability: 0.946

Residue probability confidence: 0.865

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 173.832 | 174.627 | 1.788 | 0.000 | 0.000 |
| CA 3.15.1 | 59.885 | 62.330 | 4.136 | 0.714 | 0.875 |
| CB 3.15.2 | 71.454 | 69.395 | 4.500 | 1.000 | 0.833 |
| CG2 3.15.3 | 22.007 | 21.588 | 1.595 | 1.000 | 0.833 |
| N 3.15.4 | 114.288 | 115.370 | 5.913 | 1.000 | 0.917 |
| HA 3.15.5 | 5.225 | 4.461 | 0.626 | 0.857 | 0.875 |
| HB 3.15.6 | 3.655 | 4.172 | 0.855 | 1.000 | 0.833 |
| HG2 3.15.7 | 0.557 | 1.134 | 0.349 | 1.000 | 0.833 |
| H 3.15.8 | 8.473 | 8.272 | 1.597 | 1.000 | 0.917 |
| HG1 | NA | – | – | 0.000 | 0.000 |

3.15.1 Detailed Probabilities of THR15CA:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN14 | 0.00 | 1.00 |
| THR15 | 1.00 | 0.80 |
| GLN16 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q14HA | 1.00 |
| T15HB | 1.00 |
| T15HG21 | 1.00 |
| T15H | 1.00 |
| T15HG1 | 1.00 |
| T15HA | 1.00 |
| Q16HA | 1.00 |
| Q16H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN14 | HA | 1.00 | 0.237 | 0.00 | 0.00 |
| THR15 | HA | 1.00 | 0.003 | 1.00 | 1.68 |
| THR15 | HB | 1.00 | 0.005 | 1.00 | 0.37 |
| THR15 | HG21 | 1.00 | 0.001 | 1.00 | 0.51 |
| THR15 | H | 1.00 | 0.004 | 1.00 | 0.12 |
| GLN16 | HA | 1.00 | 0.341 | 0.00 | 0.00 |
| GLN16 | H | 1.00 | 0.008 | 1.00 | 0.55 |

3.15.2 Detailed Probabilities of THR15CB:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR15 | 1.00 | 0.80 |
| GLN16 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T15HA | 1.00 |
| T15HG21 | 1.00 |
| T15H | 1.00 |
| T15HG1 | 1.00 |
| T15HB | 1.00 |
| Q16H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR15 | HA | 1.00 | 0.007 | 1.00 | 0.59 |
| THR15 | HB | 1.00 | 0.002 | 1.00 | 5.59 |
| THR15 | HG21 | 1.00 | 0.001 | 1.00 | 1.21 |
| THR15 | H | 1.00 | 0.001 | 1.00 | 0.13 |
| GLN16 | H | 1.00 | 0.008 | 1.00 | 0.45 |
| GLN16 | HA | 0.77 | 0.018 | 1.00 | 0.07 |

3.15.3 Detailed Probabilities of THR15CG2:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR15 | 1.00 | 0.80 |
| GLN16 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T15HA | 1.00 |
| T15HB | 1.00 |
| T15HG22 | 1.00 |
| T15H | 1.00 |
| T15HG1 | 1.00 |
| Q16H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR15 | HA | 1.00 | 0.005 | 1.00 | 0.57 |
| THR15 | HB | 1.00 | 0.002 | 1.00 | 2.69 |
| THR15 | HG21 | 1.00 | 0.001 | 1.00 | 63.83 |
| THR15 | H | 1.00 | 0.002 | 1.00 | 0.16 |
| GLN16 | H | 0.96 | 0.004 | 1.00 | 0.22 |

3.15.4 Detailed Probabilities of THR15N:

Overall probability: 1.000

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN14 | 1.00 | 1.00 |
| THR15 | 1.00 | 0.80 |
| GLN16 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q14HB3 | 1.00 |
| Q14H | 1.00 |
| Q14HB2 | 1.00 |
| Q14HA | 1.00 |
| Q14HG3 | 0.95 |
| Q14HG2 | 0.97 |
| T15HA | 1.00 |
| T15HB | 1.00 |
| T15HG21 | 1.00 |
| T15HG1 | 1.00 |
| T15H | 1.00 |
| Q16H | 1.00 |

NOESY contacts detailed probability

3.15 THR(15)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN14 | HA | 1.00 | 0.006 | 1.00 | -2463304.00 |
| GLN14 | HB2 | 1.00 | 0.001 | 1.00 | -771258.00 |
| GLN14 | HB3 | 1.00 | 0.002 | 1.00 | -389406.00 |
| GLN14 | HG2 | 0.97 | 0.008 | 1.00 | -257029.00 |
| GLN14 | HG3 | 0.95 | 0.009 | 1.00 | -239767.00 |
| GLN14 | H | 1.00 | 0.003 | 1.00 | -149157.00 |
| THR15 | HA | 1.00 | 0.008 | 1.00 | -441330.00 |
| THR15 | HB | 1.00 | 0.003 | 1.00 | -307710.00 |
| THR15 | HG21 | 1.00 | 0.000 | 1.00 | -554911.00 |
| THR15 | H | 1.00 | 0.001 | 1.00 | -6293334.00 |
| GLN16 | H | 1.00 | 0.001 | 1.00 | -128361.00 |
| GLN16 | HA | 0.87 | 0.004 | 1.00 | -93853.00 |
| GLN16 | HB2 | 0.56 | 0.022 | 1.00 | -389406.00 |

3.15.5 Detailed Probabilities of THR15HA:

Overall probability: 0.857

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN14 | 1.00 | 1.00 |
| THR15 | 1.00 | 0.80 |
| GLN16 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q14HA | 1.00 |
| T15HB | 1.00 |
| T15HG21 | 1.00 |
| T15H | 1.00 |
| T15HG1 | 1.00 |
| T15HA | 1.00 |
| Q16HA | 1.00 |
| Q16H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN14 | HA | 1.00 | 0.024 | 1.00 | 0.13 |
| THR15 | HA | 1.00 | 0.003 | 1.00 | 1.68 |
| THR15 | HB | 1.00 | 0.007 | 1.00 | 0.59 |
| THR15 | HG21 | 1.00 | 0.005 | 1.00 | 0.57 |
| THR15 | H | 1.00 | 0.008 | 1.00 | -441330.00 |
| GLN16 | HA | 1.00 | 0.422 | 0.00 | 0.00 |
| GLN16 | H | 1.00 | 0.007 | 1.00 | -1687766.00 |

3.15.6 Detailed Probabilities of THR15HB:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR15 | 1.00 | 0.80 |
| GLN16 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T15HA | 1.00 |
| T15HG21 | 1.00 |
| T15H | 1.00 |
| T15HG1 | 1.00 |
| T15HB | 1.00 |
| Q16H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR15 | HA | 1.00 | 0.005 | 1.00 | 0.37 |
| THR15 | HB | 1.00 | 0.002 | 1.00 | 5.59 |
| THR15 | HG21 | 1.00 | 0.002 | 1.00 | 2.69 |
| THR15 | H | 1.00 | 0.003 | 1.00 | -307710.00 |
| GLN16 | H | 1.00 | 0.003 | 1.00 | -878414.00 |
| GLN16 | HA | 0.77 | 0.013 | 1.00 | 0.07 |

3.15.7 Detailed Probabilities of THR15HG21:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR15 | 1.00 | 0.80 |
| GLN16 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T15HA | 1.00 |
| T15HB | 1.00 |
| T15HG22 | 1.00 |
| T15H | 1.00 |
| T15HG1 | 1.00 |
| Q16H | 0.97 |

NOESY contacts detailed probability

3.15 THR(15)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR15 | HA | 1.00 | 0.001 | 1.00 | 0.51 |
| THR15 | HB | 1.00 | 0.001 | 1.00 | 1.21 |
| THR15 | HG21 | 1.00 | 0.001 | 1.00 | 63.83 |
| THR15 | H | 1.00 | 0.000 | 1.00 | -554911.00 |
| GLN16 | H | 0.96 | 0.002 | 1.00 | -576923.00 |

3.15.8 Detailed Probabilities of THR15H:

Overall probability: 1.000

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN14 | 1.00 | 1.00 |
| THR15 | 1.00 | 0.80 |
| GLN16 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q14HB3 | 1.00 |
| Q14H | 1.00 |
| Q14HB2 | 1.00 |
| Q14HA | 1.00 |
| Q14HG3 | 0.95 |
| Q14HG2 | 0.97 |
| T15HA | 1.00 |
| T15HB | 1.00 |
| T15HG21 | 1.00 |
| T15HG1 | 1.00 |
| T15H | 1.00 |
| Q16H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN14 | HA | 1.00 | 0.005 | 1.00 | 1.18 |
| GLN14 | HB2 | 1.00 | 0.012 | 1.00 | 0.40 |
| GLN14 | HB3 | 1.00 | 0.028 | 1.00 | 0.37 |
| GLN14 | HG2 | 0.97 | 0.000 | 1.00 | 0.12 |
| GLN14 | HG3 | 0.95 | 0.000 | 1.00 | 0.12 |
| GLN14 | H | 1.00 | 0.000 | 1.00 | -85708.00 |
| THR15 | HA | 1.00 | 0.004 | 1.00 | 0.12 |
| THR15 | HB | 1.00 | 0.001 | 1.00 | 0.13 |
| THR15 | HG21 | 1.00 | 0.002 | 1.00 | 0.16 |
| THR15 | H | 1.00 | 0.001 | 1.00 | -6293334.00 |
| GLN16 | H | 1.00 | 0.000 | 1.00 | -94540.00 |

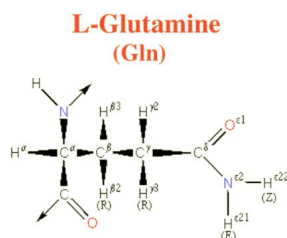
3.16 GLN(16)

Figure 6: Image from the BMRB

Residue probability: 0.877

Residue probability confidence: 0.987

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|--------------|-------------|---------|--------|---------------------|--------------------|
| C | 173.468 | 176.405 | 1.998 | 0.000 | 0.000 |
| CA 3.16.1 | 54.599 | 56.667 | 2.318 | 0.800 | 1.000 |
| CB 3.16.2 | 33.127 | 29.436 | 2.799 | 0.778 | 1.000 |
| CG 3.16.3 | 33.491 | 33.781 | 1.871 | 1.000 | 1.000 |
| N 3.16.4 | 121.949 | 119.799 | 3.762 | 1.000 | 0.917 |
| NE2 3.16.5 | 111.338 | 111.924 | 2.434 | 1.000 | 1.000 |
| HA 3.16.6 | 4.483 | 4.265 | 0.455 | 0.909 | 1.000 |
| HB2 3.16.7 | 1.902 | 2.047 | 0.290 | 0.900 | 1.000 |
| HB3 3.16.8 | 1.674 | 2.012 | 0.313 | 0.900 | 1.000 |
| HG2 3.16.9 | 2.238 | 2.308 | 0.289 | 1.000 | 1.000 |
| HG3 3.16.10 | 2.420 | 2.284 | 0.313 | 0.782 | 1.000 |
| H 3.16.11 | 8.776 | 8.232 | 0.711 | 1.000 | 0.917 |
| HE21 3.16.12 | 7.482 | 7.217 | 0.496 | 0.667 | 1.000 |
| HE22 3.16.13 | 6.804 | 7.041 | 0.463 | 0.667 | 1.000 |

3.16.1 Detailed Probabilities of GLN16CA:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR15 | 0.50 | 1.00 |
| GLN16 | 1.00 | 1.00 |
| ASP17 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T15HA | 1.00 |
| Q16HB2 | 1.00 |
| Q16HB3 | 1.00 |
| Q16HG2 | 1.00 |
| Q16HG3 | 1.00 |
| Q16H | 1.00 |
| Q16HA | 1.00 |
| D17H | 1.00 |
| D17HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR15 | HA | 1.00 | 0.422 | 0.00 | 0.00 |
| THR15 | HB | 0.77 | 0.013 | 1.00 | 0.07 |
| GLN16 | HA | 1.00 | 0.007 | 1.00 | 7.49 |
| GLN16 | HB2 | 1.00 | 0.007 | 1.00 | 0.81 |
| GLN16 | HB3 | 1.00 | 0.007 | 1.00 | 0.74 |
| GLN16 | HG2 | 1.00 | 0.005 | 1.00 | 0.52 |
| GLN16 | HG3 | 1.00 | 0.010 | 1.00 | 0.45 |
| GLN16 | H | 1.00 | 0.012 | 1.00 | 0.36 |
| ASP17 | HA | 1.00 | 0.141 | 0.00 | 0.00 |
| ASP17 | H | 1.00 | 0.001 | 1.00 | 1.85 |

3.16.2 Detailed Probabilities of GLN16CB:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN16 | 0.75 | 1.00 |
| ASP17 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q16HA | 1.00 |
| Q16HB3 | 1.00 |
| Q16HG2 | 1.00 |
| Q16HG3 | 1.00 |
| Q16H | 1.00 |
| Q16HE21 | 1.00 |
| Q16HE22 | 1.00 |
| Q16HB2 | 1.00 |
| D17H | 1.00 |

NOESY contacts detailed probability

3.16 GLN(16)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN16 | HA | 1.00 | 0.004 | 1.00 | 0.45 |
| GLN16 | HB2 | 1.00 | 0.003 | 1.00 | 4.27 |
| GLN16 | HB3 | 1.00 | 0.008 | 1.00 | 2.54 |
| GLN16 | HG2 | 1.00 | 0.002 | 1.00 | 0.77 |
| GLN16 | HG3 | 1.00 | 0.003 | 1.00 | 0.66 |
| GLN16 | H | 1.00 | 0.000 | 1.00 | 0.13 |
| GLN16 | HE21 | 1.00 | 0.591 | 0.00 | 0.00 |
| GLN16 | HE22 | 1.00 | 1.269 | 0.00 | 0.00 |
| ASP17 | H | 1.00 | 0.003 | 1.00 | 0.19 |

3.16.3 Detailed Probabilities of GLN16CG:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN16 | 1.00 | 1.00 |
| ASP17 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q16HA | 1.00 |
| Q16HB2 | 1.00 |
| Q16HB3 | 1.00 |
| Q16HG3 | 1.00 |
| Q16H | 1.00 |
| Q16HE21 | 1.00 |
| Q16HE22 | 1.00 |
| Q16HG2 | 1.00 |
| D17H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN16 | HA | 1.00 | 0.007 | 1.00 | 0.33 |
| GLN16 | HB2 | 1.00 | 0.000 | 1.00 | 0.70 |
| GLN16 | HB3 | 1.00 | 0.007 | 1.00 | 0.56 |
| GLN16 | HG2 | 1.00 | 0.012 | 1.00 | 15.17 |
| GLN16 | HG3 | 1.00 | 0.004 | 1.00 | 3.77 |
| GLN16 | H | 1.00 | 0.000 | 1.00 | 0.05 |
| GLN16 | HE21 | 1.00 | 0.024 | 1.00 | 0.21 |
| GLN16 | HE22 | 1.00 | 0.004 | 1.00 | 0.08 |
| ASP17 | H | 0.98 | 0.000 | 1.00 | 0.14 |

3.16.4 Detailed Probabilities of GLN16N:

Overall probability: 1.000

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR15 | 1.00 | 0.80 |
| GLN16 | 1.00 | 1.00 |
| ASP17 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T15HB | 1.00 |
| T15HG1 | 0.98 |
| T15HA | 1.00 |
| T15HG23 | 0.96 |
| T15H | 1.00 |
| Q16HA | 1.00 |
| Q16HB2 | 1.00 |
| Q16HB3 | 1.00 |
| Q16HG2 | 1.00 |
| Q16HG3 | 1.00 |
| Q16H | 1.00 |
| D17H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR15 | HA | 1.00 | 0.007 | 1.00 | -1687766.00 |
| THR15 | HB | 1.00 | 0.003 | 1.00 | -878414.00 |
| THR15 | HG21 | 0.97 | 0.002 | 1.00 | -576923.00 |
| THR15 | H | 1.00 | 0.000 | 1.00 | -94540.00 |
| GLN16 | HA | 1.00 | 0.006 | 1.00 | -584584.00 |
| GLN16 | HB2 | 1.00 | 0.000 | 1.00 | -552781.00 |
| GLN16 | HB3 | 1.00 | 0.019 | 1.00 | -808246.00 |
| GLN16 | HG2 | 1.00 | 0.006 | 1.00 | -136385.00 |
| GLN16 | HG3 | 1.00 | 0.001 | 1.00 | -127521.00 |
| GLN16 | H | 1.00 | 0.006 | 1.00 | -5825646.00 |
| ASP17 | H | 1.00 | 0.000 | 1.00 | -130126.00 |
| ASP17 | HA | 0.86 | 0.015 | 1.00 | -116482.00 |

3.16.5 Detailed Probabilities of GLN16NE2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN16 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q16HB2 | 1.00 |
| Q16HB3 | 1.00 |
| Q16HG2 | 1.00 |
| Q16HG3 | 1.00 |
| Q16HE22 | 1.00 |
| Q16HE21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN16 | HB2 | 1.00 | 0.006 | 1.00 | -100968.00 |
| GLN16 | HB3 | 1.00 | 0.000 | 1.00 | -98685.00 |
| GLN16 | HG2 | 1.00 | 0.000 | 1.00 | -635542.00 |
| GLN16 | HG3 | 1.00 | 0.008 | 1.00 | -548823.00 |
| GLN16 | HE21 | 1.00 | 0.003 | 1.00 | -10091628.00 |
| GLN16 | HE22 | 1.00 | 0.000 | 1.00 | -6415238.00 |

3.16.6 Detailed Probabilities of GLN16HA:

Overall probability: 0.909

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR15 | 0.67 | 1.00 |
| GLN16 | 1.00 | 1.00 |
| ASP17 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T15HA | 1.00 |
| Q16HB2 | 1.00 |
| Q16HB3 | 1.00 |
| Q16HG2 | 1.00 |
| Q16HG3 | 1.00 |
| Q16H | 1.00 |
| Q16HA | 1.00 |
| D17H | 1.00 |
| D17HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR15 | HA | 1.00 | 0.341 | 0.00 | 0.00 |
| THR15 | HB | 0.77 | 0.018 | 1.00 | 0.07 |
| THR15 | H | 0.87 | 0.004 | 1.00 | -93853.00 |
| GLN16 | HA | 1.00 | 0.007 | 1.00 | 7.49 |
| GLN16 | HB2 | 1.00 | 0.004 | 1.00 | 0.45 |
| GLN16 | HB3 | 1.00 | 0.007 | 1.00 | 0.47 |
| GLN16 | HG2 | 1.00 | 0.007 | 1.00 | 0.33 |
| GLN16 | HG3 | 1.00 | 0.006 | 1.00 | 0.36 |
| GLN16 | H | 1.00 | 0.006 | 1.00 | -584584.00 |
| ASP17 | HA | 1.00 | 0.011 | 1.00 | 0.64 |
| ASP17 | H | 1.00 | 0.006 | 1.00 | -3432666.00 |

3.16.7 Detailed Probabilities of GLN16HB2:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN16 | 0.88 | 1.00 |
| ASP17 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q16HA | 1.00 |
| Q16HB3 | 1.00 |
| Q16HG2 | 1.00 |
| Q16HG3 | 1.00 |
| Q16H | 1.00 |
| Q16HE21 | 1.00 |
| Q16HE22 | 1.00 |
| Q16HB2 | 1.00 |
| D17H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN16 | HA | 1.00 | 0.007 | 1.00 | 0.81 |
| GLN16 | HB2 | 1.00 | 0.003 | 1.00 | 4.27 |
| GLN16 | HB3 | 1.00 | 0.002 | 1.00 | 2.28 |
| GLN16 | HG2 | 1.00 | 0.000 | 1.00 | 0.70 |
| GLN16 | HG3 | 1.00 | 0.004 | 1.00 | 0.63 |
| GLN16 | H | 1.00 | 0.000 | 1.00 | -552781.00 |
| GLN16 | HE21 | 1.00 | 0.006 | 1.00 | -100968.00 |
| GLN16 | HE22 | 1.00 | 0.219 | 0.00 | 0.00 |
| ASP17 | H | 1.00 | 0.003 | 1.00 | -539830.00 |
| ASP17 | HA | 0.61 | 0.018 | 1.00 | 0.23 |

3.16.8 Detailed Probabilities of GLN16HB3:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN16 | 0.88 | 1.00 |
| ASP17 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q16HA | 1.00 |
| Q16HB2 | 1.00 |
| Q16HG2 | 1.00 |
| Q16HG3 | 1.00 |
| Q16H | 1.00 |
| Q16HE21 | 1.00 |
| Q16HE22 | 1.00 |
| Q16HB3 | 1.00 |
| D17H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN16 | HA | 1.00 | 0.007 | 1.00 | 0.74 |
| GLN16 | HB2 | 1.00 | 0.008 | 1.00 | 2.54 |
| GLN16 | HB3 | 1.00 | 0.007 | 1.00 | 4.51 |
| GLN16 | HG2 | 1.00 | 0.007 | 1.00 | 0.56 |
| GLN16 | HG3 | 1.00 | 0.004 | 1.00 | 0.59 |
| GLN16 | H | 1.00 | 0.019 | 1.00 | -808246.00 |
| GLN16 | HE21 | 1.00 | 0.000 | 1.00 | -98685.00 |
| GLN16 | HE22 | 1.00 | 0.447 | 0.00 | 0.00 |
| ASP17 | H | 1.00 | 0.009 | 1.00 | -368427.00 |
| ASP17 | HA | 0.79 | 0.025 | 1.00 | 0.31 |

3.16.9 Detailed Probabilities of GLN16HG2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN16 | 1.00 | 1.00 |
| ASP17 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q16HA | 1.00 |
| Q16HB2 | 1.00 |
| Q16HB3 | 1.00 |
| Q16HG3 | 1.00 |
| Q16H | 1.00 |
| Q16HE21 | 1.00 |
| Q16HE22 | 1.00 |
| Q16HG2 | 1.00 |
| D17H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN16 | HA | 1.00 | 0.005 | 1.00 | 0.52 |
| GLN16 | HB2 | 1.00 | 0.002 | 1.00 | 0.77 |
| GLN16 | HB3 | 1.00 | 0.001 | 1.00 | 0.51 |
| GLN16 | HG2 | 1.00 | 0.012 | 1.00 | 15.17 |
| GLN16 | HG3 | 1.00 | 0.003 | 1.00 | 3.74 |
| GLN16 | H | 1.00 | 0.006 | 1.00 | -136385.00 |
| GLN16 | HE21 | 1.00 | 0.000 | 1.00 | -635542.00 |
| GLN16 | HE22 | 1.00 | 0.005 | 1.00 | -443020.00 |
| ASP17 | H | 0.98 | 0.006 | 1.00 | -324200.00 |

3.16.10 Detailed Probabilities of GLN16HG3:

Overall probability: 0.782

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN16 | 0.88 | 1.00 |
| ASP17 | 0.04 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q16HA | 1.00 |
| Q16HB2 | 1.00 |
| Q16HB3 | 1.00 |
| Q16HG2 | 1.00 |
| Q16H | 1.00 |
| Q16HE21 | 1.00 |
| Q16HE22 | 1.00 |
| Q16HG3 | 1.00 |
| D17H | 0.96 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN16 | HA | 1.00 | 0.010 | 1.00 | 0.45 |
| GLN16 | HB2 | 1.00 | 0.003 | 1.00 | 0.66 |
| GLN16 | HB3 | 1.00 | 0.183 | 0.00 | 0.00 |
| GLN16 | HG2 | 1.00 | 0.004 | 1.00 | 3.77 |
| GLN16 | HG3 | 1.00 | 0.005 | 1.00 | 15.24 |
| GLN16 | H | 1.00 | 0.001 | 1.00 | -127521.00 |
| GLN16 | HE21 | 1.00 | 0.008 | 1.00 | -548823.00 |
| GLN16 | HE22 | 1.00 | 0.010 | 1.00 | -326499.00 |
| ASP17 | H | 0.96 | 0.081 | 0.04 | 0.00 |

3.16.11 Detailed Probabilities of GLN16H:

Overall probability: 1.000

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR15 | 1.00 | 0.80 |
| GLN16 | 1.00 | 1.00 |
| ASP17 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T15HB | 1.00 |
| T15HG1 | 0.98 |
| T15HA | 1.00 |
| T15HG23 | 0.96 |
| T15H | 1.00 |
| Q16HA | 1.00 |
| Q16HB2 | 1.00 |
| Q16HB3 | 1.00 |
| Q16HG2 | 1.00 |
| Q16HG3 | 1.00 |
| Q16H | 1.00 |
| D17H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR15 | HA | 1.00 | 0.008 | 1.00 | 0.55 |
| THR15 | HB | 1.00 | 0.008 | 1.00 | 0.45 |
| THR15 | HG21 | 0.97 | 0.004 | 1.00 | 0.22 |
| THR15 | H | 1.00 | 0.001 | 1.00 | -128361.00 |
| GLN16 | HA | 1.00 | 0.012 | 1.00 | 0.36 |
| GLN16 | HB2 | 1.00 | 0.000 | 1.00 | 0.13 |
| GLN16 | HB3 | 1.00 | 0.007 | 1.00 | 0.17 |
| GLN16 | HG2 | 1.00 | 0.000 | 1.00 | 0.05 |
| GLN16 | HG3 | 1.00 | 0.001 | 1.00 | 0.06 |
| GLN16 | H | 1.00 | 0.006 | 1.00 | -5825646.00 |
| ASP17 | H | 1.00 | 0.019 | 1.00 | -257706.00 |

3.16.12 Detailed Probabilities of GLN16HE21:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN16 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q16HB2 | 1.00 |
| Q16HB3 | 1.00 |
| Q16HG2 | 1.00 |
| Q16HG3 | 1.00 |
| Q16HE22 | 1.00 |
| Q16HE21 | 1.00 |

NOESY contacts detailed probability

3.16 GLN(16)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN16 | HB2 | 1.00 | 0.591 | 0.00 | 0.00 |
| GLN16 | HB3 | 1.00 | 0.812 | 0.00 | 0.00 |
| GLN16 | HG2 | 1.00 | 0.024 | 1.00 | 0.21 |
| GLN16 | HG3 | 1.00 | 0.007 | 1.00 | 0.20 |
| GLN16 | HE21 | 1.00 | 0.003 | 1.00 | -10091628.00 |
| GLN16 | HE22 | 1.00 | 0.002 | 1.00 | -7064521.00 |

3.16.13 Detailed Probabilities of GLN16HE22:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN16 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q16HB2 | 1.00 |
| Q16HB3 | 1.00 |
| Q16HG2 | 1.00 |
| Q16HG3 | 1.00 |
| Q16HE21 | 1.00 |
| Q16HE22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN16 | HB2 | 1.00 | 1.269 | 0.00 | 0.00 |
| GLN16 | HB3 | 1.00 | 1.490 | 0.00 | 0.00 |
| GLN16 | HG2 | 1.00 | 0.004 | 1.00 | 0.08 |
| GLN16 | HG3 | 1.00 | 0.001 | 1.00 | 0.07 |
| GLN16 | HE21 | 1.00 | 0.000 | 1.00 | -6415238.00 |
| GLN16 | HE22 | 1.00 | 0.001 | 1.00 | -11999231.00 |

3.17 ASP(17)

Figure 7: Image from the BMRB

Residue probability: 0.925

Residue probability confidence: 0.893

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 175.522 | 176.463 | 2.348 | 0.000 | 0.000 |
| CA 3.17.1 | 54.586 | 54.786 | 4.266 | 0.889 | 0.875 |
| CB 3.17.2 | 41.132 | 40.949 | 3.070 | 1.000 | 0.833 |
| N 3.17.3 | 122.736 | 120.550 | 5.690 | 0.912 | 1.000 |
| HD2 | NA | – | – | 0.000 | 0.000 |
| HA 3.17.4 | 4.617 | 4.587 | 0.329 | 0.875 | 0.875 |
| HB2 3.17.5 | 2.680 | 2.708 | 0.282 | 0.800 | 0.833 |
| HB3 3.17.6 | 2.504 | 2.654 | 0.285 | 1.000 | 0.833 |
| H 3.17.7 | 8.297 | 8.304 | 1.027 | 1.000 | 1.000 |

3.17.1 Detailed Probabilities of ASP17CA:

Overall probability: 0.889

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN16 | 1.00 | 1.00 |
| ASP17 | 1.00 | 0.80 |
| THR18 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Q16HA | 1.00 |
| D17HD2 | 1.00 |
| D17HB2 | 1.00 |
| D17HB3 | 1.00 |
| D17H | 1.00 |
| D17HA | 1.00 |
| T18HA | 1.00 |
| T18H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN16 | HA | 1.00 | 0.011 | 1.00 | 0.64 |
| GLN16 | HB2 | 0.61 | 0.018 | 1.00 | 0.23 |
| GLN16 | HB3 | 0.79 | 0.025 | 1.00 | 0.31 |
| ASP17 | HA | 1.00 | 0.007 | 1.00 | 10.54 |
| ASP17 | HB2 | 1.00 | 0.009 | 1.00 | 0.98 |
| ASP17 | HB3 | 1.00 | 0.003 | 1.00 | 0.63 |
| ASP17 | H | 1.00 | 0.003 | 1.00 | 0.53 |
| THR18 | HA | 1.00 | 0.050 | 0.00 | 0.00 |
| THR18 | H | 1.00 | 0.002 | 1.00 | 1.18 |

3.17.2 Detailed Probabilities of ASP17CB:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP17 | 1.00 | 0.80 |
| THR18 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D17HD2 | 1.00 |
| D17HA | 1.00 |
| D17HB2 | 1.00 |
| D17H | 1.00 |
| D17HB3 | 1.00 |
| T18H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP17 | HA | 1.00 | 0.006 | 1.00 | 0.63 |
| ASP17 | HB2 | 1.00 | 0.007 | 1.00 | 3.60 |
| ASP17 | HB3 | 1.00 | 0.003 | 1.00 | 4.43 |
| ASP17 | H | 1.00 | 0.001 | 1.00 | 0.51 |
| THR18 | H | 1.00 | 0.003 | 1.00 | 0.32 |
| THR18 | HA | 0.83 | 0.008 | 1.00 | 0.06 |

3.17.3 Detailed Probabilities of ASP17N:

Overall probability: 0.912

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN16 | 0.84 | 1.00 |
| ASP17 | 1.00 | 1.00 |
| THR18 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Q16HB3 | 1.00 |
| Q16HB2 | 1.00 |
| Q16H | 1.00 |
| Q16HG2 | 0.98 |
| Q16HA | 1.00 |
| Q16HG3 | 0.96 |
| D17HA | 1.00 |
| D17HB2 | 1.00 |
| D17HB3 | 1.00 |
| D17H | 1.00 |
| T18H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN16 | HA | 1.00 | 0.006 | 1.00 | -3432666.00 |
| GLN16 | HB2 | 1.00 | 0.003 | 1.00 | -539830.00 |
| GLN16 | HB3 | 1.00 | 0.009 | 1.00 | -368427.00 |
| GLN16 | HG2 | 0.98 | 0.006 | 1.00 | -324200.00 |
| GLN16 | HG3 | 0.96 | 0.081 | 0.04 | 0.00 |
| GLN16 | H | 1.00 | 0.019 | 1.00 | -257706.00 |
| ASP17 | HA | 1.00 | 0.006 | 1.00 | -710115.00 |
| ASP17 | HB2 | 1.00 | 0.006 | 1.00 | -711195.00 |
| ASP17 | HB3 | 1.00 | 0.003 | 1.00 | -1320557.00 |
| ASP17 | H | 1.00 | 0.001 | 1.00 | -8455191.00 |
| THR18 | H | 1.00 | 0.012 | 1.00 | -257706.00 |

3.17.4 Detailed Probabilities of ASP17HA:

Overall probability: 0.875

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN16 | 0.50 | 1.00 |
| ASP17 | 1.00 | 0.80 |
| THR18 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Q16HA | 1.00 |
| D17HD2 | 1.00 |
| D17HB2 | 1.00 |
| D17HB3 | 1.00 |
| D17H | 1.00 |
| D17HA | 1.00 |
| T18HA | 1.00 |
| T18H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN16 | HA | 1.00 | 0.141 | 0.00 | 0.00 |
| GLN16 | H | 0.86 | 0.015 | 1.00 | -116482.00 |
| ASP17 | HA | 1.00 | 0.007 | 1.00 | 10.54 |
| ASP17 | HB2 | 1.00 | 0.003 | 1.00 | 1.43 |
| ASP17 | HB3 | 1.00 | 0.006 | 1.00 | 0.63 |
| ASP17 | H | 1.00 | 0.006 | 1.00 | -710115.00 |
| THR18 | HA | 1.00 | 0.020 | 1.00 | 0.27 |
| THR18 | H | 1.00 | 0.007 | 1.00 | -1577892.00 |

3.17.5 Detailed Probabilities of ASP17HB2:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP17 | 0.75 | 0.80 |
| THR18 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D17HD2 | 1.00 |
| D17HA | 1.00 |
| D17HB3 | 1.00 |
| D17H | 1.00 |
| D17HB2 | 1.00 |
| T18H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP17 | HA | 1.00 | 0.009 | 1.00 | 0.98 |
| ASP17 | HB2 | 1.00 | 0.096 | 0.00 | 0.00 |
| ASP17 | HB3 | 1.00 | 0.007 | 1.00 | 3.60 |
| ASP17 | H | 1.00 | 0.006 | 1.00 | -711195.00 |
| THR18 | H | 1.00 | 0.008 | 1.00 | -691770.00 |

3.17.6 Detailed Probabilities of ASP17HB3:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP17 | 1.00 | 0.80 |
| THR18 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D17HD2 | 1.00 |
| D17HA | 1.00 |
| D17HB2 | 1.00 |
| D17H | 1.00 |
| D17HB3 | 1.00 |
| T18H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP17 | HA | 1.00 | 0.003 | 1.00 | 0.63 |
| ASP17 | HB2 | 1.00 | 0.000 | 1.00 | 4.02 |
| ASP17 | HB3 | 1.00 | 0.003 | 1.00 | 4.43 |
| ASP17 | H | 1.00 | 0.003 | 1.00 | -1320557.00 |
| THR18 | H | 1.00 | 0.004 | 1.00 | -455497.00 |

3.17.7 Detailed Probabilities of ASP17H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN16 | 1.00 | 1.00 |
| ASP17 | 1.00 | 1.00 |
| THR18 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Q16HB3 | 1.00 |
| Q16HB2 | 1.00 |
| Q16H | 1.00 |
| Q16HG2 | 0.98 |
| Q16HA | 1.00 |
| Q16HG3 | 0.96 |
| D17HA | 1.00 |
| D17HB2 | 1.00 |
| D17HB3 | 1.00 |
| D17H | 1.00 |
| T18H | 1.00 |

NOESY contacts detailed probability

3.17 ASP(17)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN16 | HA | 1.00 | 0.001 | 1.00 | 1.85 |
| GLN16 | HB2 | 1.00 | 0.003 | 1.00 | 0.19 |
| GLN16 | HB3 | 1.00 | 0.003 | 1.00 | 0.12 |
| GLN16 | HG2 | 0.98 | 0.000 | 1.00 | 0.14 |
| GLN16 | HG3 | 0.96 | 0.002 | 1.00 | 0.18 |
| GLN16 | H | 1.00 | 0.000 | 1.00 | -130126.00 |
| ASP17 | HA | 1.00 | 0.003 | 1.00 | 0.53 |
| ASP17 | HB2 | 1.00 | 0.001 | 1.00 | 0.40 |
| ASP17 | HB3 | 1.00 | 0.001 | 1.00 | 0.51 |
| ASP17 | H | 1.00 | 0.001 | 1.00 | -8455191.00 |
| THR18 | H | 1.00 | 0.000 | 1.00 | -138823.00 |

3.18 THR(18)

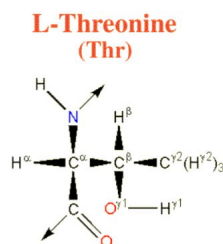


Figure 8: Image from the BMRB

Residue probability: 0.888

Residue probability confidence: 0.867

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | NA | – | – | 0.000 | 0.000 |
| CA 3.18.1 | 60.000 | 62.330 | 4.136 | 0.889 | 0.900 |
| CB 3.18.2 | 69.312 | 69.395 | 4.500 | 0.875 | 0.857 |
| CG2 3.18.3 | 20.412 | 21.588 | 1.595 | 1.000 | 0.800 |
| N 3.18.4 | 111.515 | 115.370 | 5.913 | 0.801 | 0.909 |
| HA 3.18.5 | 4.938 | 4.461 | 0.626 | 0.908 | 0.900 |
| HB 3.18.6 | 4.508 | 4.172 | 0.855 | 0.857 | 0.857 |
| HG2 3.18.7 | 1.049 | 1.134 | 0.349 | 1.000 | 0.800 |
| H 3.18.8 | 8.745 | 8.272 | 1.597 | 0.771 | 0.909 |
| HG1 | NA | – | – | 0.000 | 0.000 |

3.18.1 Detailed Probabilities of THR18CA:

Overall probability: 0.889

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP17 | 1.00 | 1.00 |
| THR18 | 0.75 | 0.80 |
| PRO19 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| D17HA | 1.00 |
| T18HB | 1.00 |
| T18HG21 | 1.00 |
| T18H | 1.00 |
| T18HG1 | 1.00 |
| T18HA | 1.00 |
| P19HD2 | 1.00 |
| P19HD3 | 1.00 |
| P19HG2 | 0.95 |
| P19HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP17 | HA | 1.00 | 0.020 | 1.00 | 0.27 |
| THR18 | HA | 1.00 | 0.004 | 1.00 | 5.02 |
| THR18 | HB | 1.00 | 0.000 | 1.00 | 0.99 |
| THR18 | HG21 | 1.00 | 0.022 | 1.00 | 1.04 |
| THR18 | H | 1.00 | 0.083 | 0.00 | 0.00 |
| PRO19 | HA | 1.00 | 0.028 | 1.00 | 0.34 |
| PRO19 | HG2 | 0.95 | 0.005 | 1.00 | 0.62 |
| PRO19 | HD2 | 1.00 | 0.004 | 1.00 | 1.19 |
| PRO19 | HD3 | 1.00 | 0.003 | 1.00 | 0.76 |

3.18.2 Detailed Probabilities of THR18CB:

Overall probability: 0.875

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR18 | 0.75 | 0.80 |
| PRO19 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T18HA | 1.00 |
| T18HG21 | 1.00 |
| T18H | 1.00 |
| T18HG1 | 1.00 |
| T18HB | 1.00 |
| P19HD3 | 0.99 |
| P19HD2 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR18 | HA | 1.00 | 0.009 | 1.00 | 0.99 |
| THR18 | HB | 1.00 | 0.136 | 0.00 | 0.00 |
| THR18 | HG21 | 1.00 | 0.005 | 1.00 | 1.21 |
| THR18 | H | 1.00 | 0.015 | 1.00 | 0.12 |
| PRO19 | HD2 | 0.99 | 0.002 | 1.00 | 0.73 |
| PRO19 | HD3 | 0.99 | 0.007 | 1.00 | 1.10 |
| PRO19 | HG2 | 0.58 | 0.002 | 1.00 | 0.17 |
| PRO19 | HG3 | 0.52 | 0.025 | 1.00 | 0.14 |

3.18.3 Detailed Probabilities of THR18CG2:

Overall probability: 1.000

Overall confidence: 0.800

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR18 | 1.00 | 0.80 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T18HA | 1.00 |
| T18HB | 1.00 |
| T18HG22 | 1.00 |
| T18H | 1.00 |
| T18HG1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR18 | HA | 1.00 | 0.001 | 1.00 | 1.32 |
| THR18 | HB | 1.00 | 0.013 | 1.00 | 2.11 |
| THR18 | HG21 | 1.00 | 0.006 | 1.00 | 55.38 |
| THR18 | H | 1.00 | 0.005 | 1.00 | 0.87 |

3.18.4 Detailed Probabilities of THR18N:

Overall probability: 0.801

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP17 | 1.00 | 1.00 |
| THR18 | 1.00 | 0.80 |
| PRO19 | 0.01 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| D17H | 1.00 |
| D17HA | 1.00 |
| D17HB2 | 1.00 |
| D17HB3 | 1.00 |
| T18HA | 1.00 |
| T18HB | 1.00 |
| T18HG21 | 1.00 |
| T18HG1 | 1.00 |
| T18H | 1.00 |
| P19HD2 | 1.00 |
| P19HD3 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP17 | HA | 1.00 | 0.007 | 1.00 | -1577892.00 |
| ASP17 | HB2 | 1.00 | 0.008 | 1.00 | -691770.00 |
| ASP17 | HB3 | 1.00 | 0.004 | 1.00 | -455497.00 |
| ASP17 | H | 1.00 | 0.000 | 1.00 | -138823.00 |
| THR18 | HA | 1.00 | 0.001 | 1.00 | -327620.00 |
| THR18 | HB | 1.00 | 0.014 | 1.00 | -176466.00 |
| THR18 | HG21 | 1.00 | 0.006 | 1.00 | -621092.00 |
| THR18 | H | 1.00 | 0.005 | 1.00 | -4237646.00 |
| PRO19 | HD2 | 1.00 | 0.649 | 0.00 | 0.00 |
| PRO19 | HD3 | 0.99 | 0.878 | 0.01 | 0.00 |

3.18.5 Detailed Probabilities of THR18HA:

Overall probability: 0.908

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP17 | 0.67 | 1.00 |
| THR18 | 1.00 | 0.80 |
| PRO19 | 0.98 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| D17HA | 1.00 |
| T18HB | 1.00 |
| T18HG21 | 1.00 |
| T18H | 1.00 |
| T18HG1 | 1.00 |
| T18HA | 1.00 |
| P19HD2 | 1.00 |
| P19HD3 | 1.00 |
| P19HG2 | 0.95 |
| P19HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP17 | HA | 1.00 | 0.050 | 0.00 | 0.00 |
| ASP17 | HB2 | 0.51 | 0.020 | 1.00 | 0.06 |
| ASP17 | HB3 | 0.83 | 0.008 | 1.00 | 0.06 |
| THR18 | HA | 1.00 | 0.004 | 1.00 | 5.02 |
| THR18 | HB | 1.00 | 0.009 | 1.00 | 0.99 |
| THR18 | HG21 | 1.00 | 0.001 | 1.00 | 1.32 |
| THR18 | H | 1.00 | 0.001 | 1.00 | -327620.00 |
| PRO19 | HA | 1.00 | 0.031 | 0.90 | 0.00 |
| PRO19 | HG2 | 0.95 | 0.006 | 1.00 | 0.18 |
| PRO19 | HD2 | 1.00 | 0.001 | 1.00 | 0.99 |
| PRO19 | HD3 | 1.00 | 0.002 | 1.00 | 0.69 |
| PRO19 | HG3 | 0.94 | 0.005 | 1.00 | 0.16 |

3.18.6 Detailed Probabilities of THR18HB:

Overall probability: 0.857

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR18 | 0.75 | 0.80 |
| PRO19 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T18HA | 1.00 |
| T18HG21 | 1.00 |
| T18H | 1.00 |
| T18HG1 | 1.00 |
| T18HB | 1.00 |
| P19HD3 | 0.99 |
| P19HD2 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR18 | HA | 1.00 | 0.000 | 1.00 | 0.99 |
| THR18 | HB | 1.00 | 0.136 | 0.00 | 0.00 |
| THR18 | HG21 | 1.00 | 0.013 | 1.00 | 2.11 |
| THR18 | H | 1.00 | 0.014 | 1.00 | -176466.00 |
| PRO19 | HD2 | 0.99 | 0.001 | 1.00 | 0.70 |
| PRO19 | HD3 | 0.99 | 0.000 | 1.00 | 0.85 |
| PRO19 | HG2 | 0.58 | 0.003 | 1.00 | 0.51 |

3.18.7 Detailed Probabilities of THR18HG21:

Overall probability: 1.000

Overall confidence: 0.800

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR18 | 1.00 | 0.80 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T18HA | 1.00 |
| T18HB | 1.00 |
| T18HG22 | 1.00 |
| T18H | 1.00 |
| T18HG1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR18 | HA | 1.00 | 0.022 | 1.00 | 1.04 |
| THR18 | HB | 1.00 | 0.005 | 1.00 | 1.21 |
| THR18 | HG21 | 1.00 | 0.006 | 1.00 | 55.38 |
| THR18 | H | 1.00 | 0.006 | 1.00 | -621092.00 |

3.18.8 Detailed Probabilities of THR18H:

Overall probability: 0.771

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP17 | 1.00 | 1.00 |
| THR18 | 0.75 | 0.80 |
| PRO19 | 0.35 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| D17H | 1.00 |
| D17HA | 1.00 |
| D17HB2 | 1.00 |
| D17HB3 | 1.00 |
| T18HA | 1.00 |
| T18HB | 1.00 |
| T18HG21 | 1.00 |
| T18HG1 | 1.00 |
| T18H | 1.00 |
| P19HD2 | 1.00 |
| P19HD3 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP17 | HA | 1.00 | 0.002 | 1.00 | 1.18 |
| ASP17 | HB2 | 1.00 | 0.006 | 1.00 | 0.50 |
| ASP17 | HB3 | 1.00 | 0.003 | 1.00 | 0.32 |
| ASP17 | H | 1.00 | 0.012 | 1.00 | -257706.00 |
| THR18 | HA | 1.00 | 0.083 | 0.00 | 0.00 |
| THR18 | HB | 1.00 | 0.015 | 1.00 | 0.12 |
| THR18 | HG21 | 1.00 | 0.005 | 1.00 | 0.87 |
| THR18 | H | 1.00 | 0.005 | 1.00 | -4237646.00 |
| PRO19 | HD2 | 1.00 | 0.033 | 0.70 | 0.00 |
| PRO19 | HD3 | 0.99 | 0.907 | 0.01 | 0.00 |

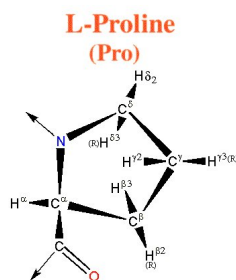
3.19 PRO(19)

Figure 9: Image from the BMRB

Residue probability: 0.696

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 175.808 | 175.173 | 13.901 | 0.000 | 0.000 |
| CA 3.19.1 | 63.908 | 62.931 | 15.301 | 0.890 | 1.000 |
| CB 3.19.2 | 31.760 | 33.632 | 13.629 | 0.625 | 1.000 |
| CG 3.19.3 | 27.613 | 28.412 | 13.801 | 0.800 | 1.000 |
| CD 3.19.4 | 50.991 | 49.797 | 3.175 | 0.791 | 1.000 |
| N | NA | - | - | 0.000 | 0.000 |
| HA 3.19.5 | 4.396 | 4.332 | 0.427 | 0.700 | 1.000 |
| HB2 3.19.6 | 1.831 | 2.099 | 0.501 | 0.491 | 1.000 |
| HB3 3.19.7 | 2.453 | 2.052 | 0.596 | 0.875 | 1.000 |
| HG2 3.19.8 | 2.032 | 1.927 | 0.364 | 0.511 | 1.000 |
| HG3 3.19.9 | 1.885 | 1.907 | 0.417 | 0.429 | 1.000 |
| HD2 3.19.10 | 3.845 | 3.640 | 0.682 | 0.819 | 1.000 |
| HD3 3.19.11 | 3.616 | 3.558 | 0.522 | 0.728 | 1.000 |

3.19.1 Detailed Probabilities of PRO19CA:

Overall probability: 0.890

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR18 | 0.90 | 1.00 |
| PRO19 | 0.86 | 1.00 |
| ASN20 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T18HA | 1.00 |
| P19HB2 | 1.00 |
| P19HB3 | 1.00 |
| P19HG2 | 1.00 |
| P19HG3 | 1.00 |
| P19HD2 | 1.00 |
| P19HD3 | 1.00 |
| P19HA | 1.00 |
| N20H | 1.00 |
| N20HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR18 | HA | 1.00 | 0.031 | 0.90 | 0.00 |
| PRO19 | HA | 1.00 | 0.005 | 1.00 | 10.96 |
| PRO19 | HB2 | 1.00 | 0.014 | 1.00 | 1.06 |
| PRO19 | HB3 | 1.00 | 0.009 | 1.00 | 1.51 |
| PRO19 | HG2 | 1.00 | 0.003 | 1.00 | 0.27 |
| PRO19 | HG3 | 1.00 | 0.040 | 0.00 | 0.00 |
| PRO19 | HD2 | 1.00 | 0.026 | 1.00 | 0.65 |
| PRO19 | HD3 | 1.00 | 0.000 | 1.00 | 0.18 |
| ASN20 | HA | 1.00 | 0.022 | 1.00 | 0.05 |
| ASN20 | H | 1.00 | 0.007 | 1.00 | 0.17 |

3.19.2 Detailed Probabilities of PRO19CB:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO19 | 0.57 | 1.00 |
| ASN20 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P19HA | 1.00 |
| P19HB2 | 1.00 |
| P19HG2 | 1.00 |
| P19HG3 | 1.00 |
| P19HD2 | 1.00 |
| P19HD3 | 1.00 |
| P19HB3 | 1.00 |
| N20H | 1.00 |

NOESY contacts detailed probability

3.19 PRO(19)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO19 | HA | 1.00 | 0.006 | 1.00 | 1.01 |
| PRO19 | HB2 | 1.00 | 0.006 | 1.00 | 2.42 |
| PRO19 | HB3 | 1.00 | 0.616 | 0.00 | 0.00 |
| PRO19 | HG2 | 1.00 | 0.195 | 0.00 | 0.00 |
| PRO19 | HG3 | 1.00 | 0.048 | 0.00 | 0.00 |
| PRO19 | HD2 | 1.00 | 0.005 | 1.00 | 0.17 |
| PRO19 | HD3 | 1.00 | 0.001 | 1.00 | 0.20 |
| ASN20 | H | 1.00 | 0.012 | 1.00 | 0.08 |

3.19.3 Detailed Probabilities of PRO19CG:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO19 | 0.80 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P19HA | 1.00 |
| P19HB2 | 1.00 |
| P19HB3 | 1.00 |
| P19HG2 | 1.00 |
| P19HD2 | 1.00 |
| P19HD3 | 1.00 |
| P19HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO19 | HA | 1.00 | 0.022 | 1.00 | 0.54 |
| PRO19 | HB2 | 1.00 | 0.058 | 0.00 | 0.00 |
| PRO19 | HB3 | 1.00 | 0.012 | 1.00 | 0.79 |
| PRO19 | HG2 | 1.00 | 0.034 | 0.60 | 0.00 |
| PRO19 | HG3 | 1.00 | 0.004 | 1.00 | 9.37 |
| PRO19 | HD2 | 1.00 | 0.013 | 1.00 | 0.90 |
| PRO19 | HD3 | 1.00 | 0.003 | 1.00 | 0.48 |

3.19.4 Detailed Probabilities of PRO19CD:

Overall probability: 0.791

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR18 | 0.93 | 1.00 |
| PRO19 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T18H | 1.00 |
| T18HB | 0.99 |
| T18HA | 1.00 |
| P19HA | 1.00 |
| P19HB2 | 1.00 |
| P19HB3 | 1.00 |
| P19HG2 | 1.00 |
| P19HG3 | 1.00 |
| P19HD3 | 1.00 |
| P19HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR18 | HA | 1.00 | 0.001 | 1.00 | 0.99 |
| THR18 | HB | 0.99 | 0.001 | 1.00 | 0.70 |
| THR18 | H | 1.00 | 0.033 | 0.70 | 0.00 |
| THR18 | HG21 | 0.94 | 0.005 | 1.00 | 0.30 |
| PRO19 | HA | 1.00 | 0.111 | 0.00 | 0.00 |
| PRO19 | HB2 | 1.00 | 0.045 | 0.00 | 0.00 |
| PRO19 | HB3 | 1.00 | 0.011 | 1.00 | 0.15 |
| PRO19 | HG2 | 1.00 | 0.023 | 1.00 | 0.64 |
| PRO19 | HG3 | 1.00 | 0.009 | 1.00 | 0.45 |
| PRO19 | HD2 | 1.00 | 0.012 | 1.00 | 3.82 |
| PRO19 | HD3 | 1.00 | 0.002 | 1.00 | 1.61 |

3.19.5 Detailed Probabilities of PRO19HA:

Overall probability: 0.700

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR18 | 1.00 | 1.00 |
| PRO19 | 0.71 | 1.00 |
| ASN20 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T18HA | 1.00 |
| P19HB2 | 1.00 |
| P19HB3 | 1.00 |
| P19HG2 | 1.00 |
| P19HG3 | 1.00 |
| P19HD2 | 1.00 |
| P19HD3 | 1.00 |
| P19HA | 1.00 |
| N20H | 1.00 |
| N20HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR18 | HA | 1.00 | 0.028 | 1.00 | 0.34 |
| PRO19 | HA | 1.00 | 0.005 | 1.00 | 10.96 |
| PRO19 | HB2 | 1.00 | 0.016 | 1.00 | 0.72 |
| PRO19 | HB3 | 1.00 | 0.006 | 1.00 | 1.01 |
| PRO19 | HG2 | 1.00 | 0.010 | 1.00 | 0.44 |
| PRO19 | HG3 | 1.00 | 0.022 | 1.00 | 0.54 |
| PRO19 | HD2 | 1.00 | 0.111 | 0.00 | 0.00 |
| PRO19 | HD3 | 1.00 | 0.112 | 0.00 | 0.00 |
| ASN20 | HA | 1.00 | 0.103 | 0.00 | 0.00 |
| ASN20 | H | 1.00 | 0.006 | 1.00 | -344809.00 |

3.19.6 Detailed Probabilities of PRO19HB2:

Overall probability: 0.491

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO19 | 0.49 | 1.00 |
| ASN20 | 0.51 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P19HA | 1.00 |
| P19HB3 | 1.00 |
| P19HG2 | 1.00 |
| P19HG3 | 1.00 |
| P19HD2 | 1.00 |
| P19HD3 | 1.00 |
| P19HB2 | 1.00 |
| N20HA | 0.98 |
| N20H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO19 | HA | 1.00 | 0.014 | 1.00 | 1.06 |
| PRO19 | HB2 | 1.00 | 0.005 | 1.00 | 6.97 |
| PRO19 | HB3 | 1.00 | 0.006 | 1.00 | 2.42 |
| PRO19 | HG2 | 1.00 | 0.115 | 0.00 | 0.00 |
| PRO19 | HG3 | 1.00 | 0.058 | 0.00 | 0.00 |
| PRO19 | HD2 | 1.00 | 0.045 | 0.00 | 0.00 |
| PRO19 | HD3 | 1.00 | 0.036 | 0.40 | 0.00 |
| ASN20 | HA | 0.98 | 0.043 | 0.02 | 0.00 |
| ASN20 | H | 1.00 | 0.003 | 1.00 | -225279.00 |

3.19.7 Detailed Probabilities of PRO19HB3:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO19 | 0.86 | 1.00 |
| ASN20 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P19HA | 1.00 |
| P19HB2 | 1.00 |
| P19HG2 | 1.00 |
| P19HG3 | 1.00 |
| P19HD2 | 1.00 |
| P19HD3 | 1.00 |
| P19HB3 | 1.00 |
| N20H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO19 | HA | 1.00 | 0.009 | 1.00 | 1.51 |
| PRO19 | HB2 | 1.00 | 0.012 | 1.00 | 1.79 |
| PRO19 | HB3 | 1.00 | 0.616 | 0.00 | 0.00 |
| PRO19 | HG2 | 1.00 | 0.014 | 1.00 | 0.75 |
| PRO19 | HG3 | 1.00 | 0.012 | 1.00 | 0.79 |
| PRO19 | HD2 | 1.00 | 0.011 | 1.00 | 0.15 |
| PRO19 | HD3 | 1.00 | 0.006 | 1.00 | 0.14 |
| ASN20 | H | 1.00 | 0.005 | 1.00 | -182085.00 |

3.19.8 Detailed Probabilities of PRO19HG2:

Overall probability: 0.511

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR18 | 1.00 | 1.00 |
| PRO19 | 0.37 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T18HA | 0.95 |
| P19HA | 1.00 |
| P19HB2 | 1.00 |
| P19HB3 | 1.00 |
| P19HG3 | 1.00 |
| P19HD2 | 1.00 |
| P19HD3 | 1.00 |
| P19HG2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR18 | HA | 0.95 | 0.005 | 1.00 | 0.62 |
| THR18 | HB | 0.58 | 0.002 | 1.00 | 0.17 |
| PRO19 | HA | 1.00 | 0.003 | 1.00 | 0.27 |
| PRO19 | HB2 | 1.00 | 0.042 | 0.00 | 0.00 |
| PRO19 | HB3 | 1.00 | 0.195 | 0.00 | 0.00 |
| PRO19 | HG2 | 1.00 | 0.316 | 0.00 | 0.00 |
| PRO19 | HG3 | 1.00 | 0.034 | 0.60 | 0.00 |
| PRO19 | HD2 | 1.00 | 0.023 | 1.00 | 0.64 |
| PRO19 | HD3 | 1.00 | 0.165 | 0.00 | 0.00 |

3.19.9 Detailed Probabilities of PRO19HG3:

Overall probability: 0.429

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO19 | 0.43 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P19HA | 1.00 |
| P19HB2 | 1.00 |
| P19HB3 | 1.00 |
| P19HG2 | 1.00 |
| P19HD2 | 1.00 |
| P19HD3 | 1.00 |
| P19HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO19 | HA | 1.00 | 0.040 | 0.00 | 0.00 |
| PRO19 | HB2 | 1.00 | 0.059 | 0.00 | 0.00 |
| PRO19 | HB3 | 1.00 | 0.048 | 0.00 | 0.00 |
| PRO19 | HG2 | 1.00 | 0.169 | 0.00 | 0.00 |
| PRO19 | HG3 | 1.00 | 0.004 | 1.00 | 9.37 |
| PRO19 | HD2 | 1.00 | 0.009 | 1.00 | 0.45 |
| PRO19 | HD3 | 1.00 | 0.018 | 1.00 | 0.44 |

3.19.10 Detailed Probabilities of PRO19HD2:

Overall probability: 0.819

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR18 | 0.75 | 1.00 |
| PRO19 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T18H | 1.00 |
| T18HB | 0.99 |
| T18HA | 1.00 |
| P19HA | 1.00 |
| P19HB2 | 1.00 |
| P19HB3 | 1.00 |
| P19HG2 | 1.00 |
| P19HG3 | 1.00 |
| P19HD3 | 1.00 |
| P19HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR18 | HA | 1.00 | 0.004 | 1.00 | 1.19 |
| THR18 | HB | 0.99 | 0.002 | 1.00 | 0.73 |
| THR18 | H | 1.00 | 0.649 | 0.00 | 0.00 |
| THR18 | HG21 | 0.94 | 0.004 | 1.00 | 0.37 |
| PRO19 | HA | 1.00 | 0.026 | 1.00 | 0.65 |
| PRO19 | HB2 | 1.00 | 0.017 | 1.00 | 0.29 |
| PRO19 | HB3 | 1.00 | 0.005 | 1.00 | 0.17 |
| PRO19 | HG2 | 1.00 | 0.047 | 0.00 | 0.00 |
| PRO19 | HG3 | 1.00 | 0.013 | 1.00 | 0.90 |
| PRO19 | HD2 | 1.00 | 0.012 | 1.00 | 3.82 |
| PRO19 | HD3 | 1.00 | 0.005 | 1.00 | 1.69 |

3.19.11 Detailed Probabilities of PRO19HD3:

Overall probability: 0.728

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR18 | 0.75 | 1.00 |
| PRO19 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T18HB | 0.99 |
| T18H | 0.99 |
| T18HA | 1.00 |
| P19HA | 1.00 |
| P19HB2 | 1.00 |
| P19HB3 | 1.00 |
| P19HG2 | 1.00 |
| P19HG3 | 1.00 |
| P19HD2 | 1.00 |
| P19HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR18 | HA | 1.00 | 0.003 | 1.00 | 0.76 |
| THR18 | HB | 0.99 | 0.007 | 1.00 | 1.10 |
| THR18 | H | 0.99 | 0.878 | 0.01 | 0.00 |
| THR18 | HG21 | 0.79 | 0.005 | 1.00 | 0.77 |
| PRO19 | HA | 1.00 | 0.000 | 1.00 | 0.18 |
| PRO19 | HB2 | 1.00 | 0.045 | 0.00 | 0.00 |
| PRO19 | HB3 | 1.00 | 0.001 | 1.00 | 0.20 |
| PRO19 | HG2 | 1.00 | 0.021 | 1.00 | 1.62 |
| PRO19 | HG3 | 1.00 | 0.003 | 1.00 | 0.48 |
| PRO19 | HD2 | 1.00 | 0.002 | 1.00 | 1.61 |
| PRO19 | HD3 | 1.00 | 0.224 | 0.00 | 0.00 |

3.20 ASN(20)

Figure 10: Image from the BMRB

Residue probability: 0.833

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|--------------|-------------|---------|--------|---------------------|--------------------|
| C | NA | – | – | 0.000 | 0.000 |
| CA 3.20.1 | 49.292 | 53.674 | 5.429 | 0.548 | 1.000 |
| CB 3.20.2 | 40.042 | 38.785 | 5.449 | 0.914 | 1.000 |
| N 3.20.3 | 116.237 | 118.907 | 6.480 | 0.925 | 1.000 |
| ND2 3.20.4 | 112.700 | 112.932 | 14.355 | 1.000 | 1.000 |
| HA 3.20.5 | 5.185 | 4.658 | 0.371 | 0.859 | 1.000 |
| HB2 3.20.6 | 2.911 | 2.800 | 0.341 | 0.857 | 1.000 |
| HB3 3.20.7 | 2.673 | 2.739 | 0.364 | 1.000 | 1.000 |
| H 3.20.8 | 7.831 | 8.328 | 0.633 | 0.875 | 1.000 |
| HD21 3.20.9 | 7.245 | 7.343 | 1.188 | 0.671 | 1.000 |
| HD22 3.20.10 | 7.603 | 7.145 | 1.184 | 0.680 | 1.000 |

3.20.1 Detailed Probabilities of ASN20CA:

Overall probability: 0.548

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO19 | 0.34 | 1.00 |
| ASN20 | 0.67 | 1.00 |
| PRO21 | 0.53 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P19HB2 | 0.98 |
| P19HA | 1.00 |
| N20HB2 | 1.00 |
| N20HB3 | 1.00 |
| N20H | 1.00 |
| N20HD21 | 1.00 |
| N20HD22 | 1.00 |
| N20HA | 1.00 |
| P21HA | 1.00 |
| P21HG2 | 0.95 |
| P21HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO19 | HA | 1.00 | 0.103 | 0.00 | 0.00 |
| PRO19 | HB2 | 0.98 | 0.043 | 0.02 | 0.00 |
| PRO19 | HG2 | 0.65 | 0.020 | 1.00 | 0.37 |
| ASN20 | HA | 1.00 | 0.000 | 1.00 | 6.14 |
| ASN20 | HB2 | 1.00 | 0.006 | 1.00 | 0.41 |
| ASN20 | HB3 | 1.00 | 0.001 | 1.00 | 0.68 |
| ASN20 | H | 1.00 | 0.005 | 1.00 | 0.31 |
| ASN20 | HD21 | 1.00 | 0.043 | 0.00 | 0.00 |
| ASN20 | HD22 | 1.00 | 0.084 | 0.00 | 0.00 |
| PRO21 | HA | 1.00 | 0.053 | 0.00 | 0.00 |
| PRO21 | HG2 | 0.95 | 0.039 | 0.10 | 0.00 |
| PRO21 | HD2 | 1.00 | 0.001 | 1.00 | 3.00 |
| PRO21 | HG3 | 0.93 | 0.007 | 1.00 | 0.37 |

3.20.2 Detailed Probabilities of ASN20CB:

Overall probability: 0.914

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN20 | 0.90 | 1.00 |
| PRO21 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N20HA | 1.00 |
| N20HB3 | 1.00 |
| N20H | 1.00 |
| N20HD21 | 1.00 |
| N20HD22 | 1.00 |
| N20HB2 | 1.00 |
| P21HD3 | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN20 | HA | 1.00 | 0.001 | 1.00 | 0.44 |
| ASN20 | HB2 | 1.00 | 0.001 | 1.00 | 6.04 |
| ASN20 | HB3 | 1.00 | 0.001 | 1.00 | 2.26 |
| ASN20 | H | 1.00 | 0.005 | 1.00 | 0.36 |
| ASN20 | HD21 | 1.00 | 0.010 | 1.00 | 0.11 |
| ASN20 | HD22 | 1.00 | 0.036 | 0.40 | 0.00 |
| PRO21 | HD2 | 0.98 | 0.003 | 1.00 | 0.22 |

3.20.3 Detailed Probabilities of ASN20N:

Overall probability: 0.925

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO19 | 1.00 | 1.00 |
| ASN20 | 0.80 | 1.00 |
| PRO21 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P19HB2 | 1.00 |
| P19HA | 1.00 |
| P19HB3 | 1.00 |
| N20HA | 1.00 |
| N20HB2 | 1.00 |
| N20HB3 | 1.00 |
| N20HD21 | 0.98 |
| N20H | 1.00 |
| P21HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO19 | HA | 1.00 | 0.006 | 1.00 | -344809.00 |
| PRO19 | HB2 | 1.00 | 0.003 | 1.00 | -225279.00 |
| PRO19 | HB3 | 1.00 | 0.005 | 1.00 | -182085.00 |
| PRO19 | HG2 | 0.95 | 0.002 | 1.00 | -163087.00 |
| PRO19 | HD2 | 0.77 | 0.001 | 1.00 | -198999.00 |
| PRO19 | HD3 | 0.71 | 0.001 | 1.00 | -431406.00 |
| ASN20 | HA | 1.00 | 0.003 | 1.00 | -777975.00 |
| ASN20 | HB2 | 1.00 | 0.004 | 1.00 | -994890.00 |
| ASN20 | HB3 | 1.00 | 0.002 | 1.00 | -899441.00 |
| ASN20 | H | 1.00 | 0.003 | 1.00 | -6714740.00 |
| ASN20 | HD21 | 0.98 | 0.589 | 0.02 | 0.00 |
| PRO21 | HD2 | 1.00 | 0.001 | 1.00 | -282499.00 |
| PRO21 | HA | 0.76 | 0.006 | 1.00 | -134878.00 |

3.20.4 Detailed Probabilities of ASN20ND2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN20 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N20HA | 1.00 |
| N20HB2 | 1.00 |
| N20HB3 | 1.00 |
| N20HD21 | 1.00 |
| N20HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN20 | HA | 1.00 | 0.018 | 1.00 | -90335.00 |
| ASN20 | HB2 | 1.00 | 0.007 | 1.00 | -141103.00 |
| ASN20 | HB3 | 1.00 | 0.001 | 1.00 | -176629.00 |
| ASN20 | HD21 | 1.00 | 0.004 | 1.00 | -1326578.00 |
| ASN20 | HD22 | 1.00 | 0.013 | 1.00 | -474376.00 |

3.20.5 Detailed Probabilities of ASN20HA:

Overall probability: 0.859

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO19 | 0.67 | 1.00 |
| ASN20 | 0.83 | 1.00 |
| PRO21 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P19HB2 | 0.98 |
| P19HA | 1.00 |
| N20HB2 | 1.00 |
| N20HB3 | 1.00 |
| N20H | 1.00 |
| N20HD21 | 1.00 |
| N20HD22 | 1.00 |
| N20HA | 1.00 |
| P21HA | 1.00 |
| P21HG2 | 0.95 |
| P21HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO19 | HA | 1.00 | 0.022 | 1.00 | 0.05 |
| PRO19 | HB2 | 0.98 | 0.260 | 0.02 | 0.00 |
| PRO19 | HG2 | 0.65 | 0.000 | 1.00 | 0.32 |
| ASN20 | HA | 1.00 | 0.000 | 1.00 | 6.14 |
| ASN20 | HB2 | 1.00 | 0.001 | 1.00 | 0.44 |
| ASN20 | HB3 | 1.00 | 0.001 | 1.00 | 0.62 |
| ASN20 | H | 1.00 | 0.003 | 1.00 | -777975.00 |
| ASN20 | HD21 | 1.00 | 0.387 | 0.00 | 0.00 |
| ASN20 | HD22 | 1.00 | 0.018 | 1.00 | -90335.00 |
| PRO21 | HA | 1.00 | 0.015 | 1.00 | 0.12 |
| PRO21 | HG2 | 0.95 | 0.001 | 1.00 | 0.27 |
| PRO21 | HD2 | 1.00 | 0.001 | 1.00 | 1.81 |
| PRO21 | HB3 | 0.80 | 0.001 | 1.00 | 0.15 |
| PRO21 | HG3 | 0.93 | 0.000 | 1.00 | 0.32 |

3.20.6 Detailed Probabilities of ASN20HB2:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN20 | 0.83 | 1.00 |
| PRO21 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N20HA | 1.00 |
| N20HB3 | 1.00 |
| N20H | 1.00 |
| N20HD21 | 1.00 |
| N20HD22 | 1.00 |
| N20HB2 | 1.00 |
| P21HD3 | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN20 | HA | 1.00 | 0.006 | 1.00 | 0.41 |
| ASN20 | HB2 | 1.00 | 0.001 | 1.00 | 6.04 |
| ASN20 | HB3 | 1.00 | 0.047 | 0.00 | 0.00 |
| ASN20 | H | 1.00 | 0.004 | 1.00 | -994890.00 |
| ASN20 | HD21 | 1.00 | 0.009 | 1.00 | -159970.00 |
| ASN20 | HD22 | 1.00 | 0.007 | 1.00 | -141103.00 |
| PRO21 | HD2 | 0.98 | 0.000 | 1.00 | 0.10 |

3.20.7 Detailed Probabilities of ASN20HB3:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN20 | 1.00 | 1.00 |
| PRO21 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N20HA | 1.00 |
| N20HB2 | 1.00 |
| N20H | 1.00 |
| N20HD21 | 1.00 |
| N20HD22 | 1.00 |
| N20HB3 | 1.00 |
| P21HD2 | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN20 | HA | 1.00 | 0.001 | 1.00 | 0.68 |
| ASN20 | HB2 | 1.00 | 0.001 | 1.00 | 2.26 |
| ASN20 | HB3 | 1.00 | 0.015 | 1.00 | 11.11 |
| ASN20 | H | 1.00 | 0.002 | 1.00 | -899441.00 |
| ASN20 | HD21 | 1.00 | 0.002 | 1.00 | -263981.00 |
| ASN20 | HD22 | 1.00 | 0.001 | 1.00 | -176629.00 |
| PRO21 | HD2 | 0.98 | 0.006 | 1.00 | 0.16 |

3.20.8 Detailed Probabilities of ASN20H:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO19 | 0.92 | 1.00 |
| ASN20 | 0.80 | 1.00 |
| PRO21 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P19HB2 | 1.00 |
| P19HA | 1.00 |
| P19HB3 | 1.00 |
| N20HA | 1.00 |
| N20HB2 | 1.00 |
| N20HB3 | 1.00 |
| N20HD21 | 0.98 |
| N20H | 1.00 |
| P21HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO19 | HA | 1.00 | 0.007 | 1.00 | 0.17 |
| PRO19 | HB2 | 1.00 | 0.034 | 0.60 | 0.00 |
| PRO19 | HB3 | 1.00 | 0.012 | 1.00 | 0.08 |
| PRO19 | HD2 | 0.77 | 0.021 | 1.00 | 0.06 |
| PRO19 | HD3 | 0.71 | 0.007 | 1.00 | 0.08 |
| ASN20 | HA | 1.00 | 0.005 | 1.00 | 0.31 |
| ASN20 | HB2 | 1.00 | 0.005 | 1.00 | 0.36 |
| ASN20 | HB3 | 1.00 | 0.006 | 1.00 | 0.37 |
| ASN20 | H | 1.00 | 0.003 | 1.00 | -6714740.00 |
| ASN20 | HD21 | 0.98 | 0.227 | 0.02 | 0.00 |
| PRO21 | HD2 | 1.00 | 0.004 | 1.00 | 0.05 |

3.20.9 Detailed Probabilities of ASN20HD21:

Overall probability: 0.671

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN20 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N20HA | 1.00 |
| N20HB2 | 1.00 |
| N20HB3 | 1.00 |
| N20H | 0.98 |
| N20HD22 | 1.00 |
| N20HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN20 | HA | 1.00 | 0.043 | 0.00 | 0.00 |
| ASN20 | HB2 | 1.00 | 0.010 | 1.00 | 0.11 |
| ASN20 | HB3 | 1.00 | 0.006 | 1.00 | 0.10 |
| ASN20 | H | 0.98 | 0.589 | 0.02 | 0.00 |
| ASN20 | HD21 | 1.00 | 0.004 | 1.00 | -3874631.00 |
| ASN20 | HD22 | 1.00 | 0.004 | 1.00 | -1326578.00 |

3.20.10 Detailed Probabilities of ASN20HD22:

Overall probability: 0.680

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN20 | 0.68 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N20HA | 1.00 |
| N20HB2 | 1.00 |
| N20HB3 | 1.00 |
| N20HD21 | 1.00 |
| N20HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN20 | HA | 1.00 | 0.084 | 0.00 | 0.00 |
| ASN20 | HB2 | 1.00 | 0.036 | 0.40 | 0.00 |
| ASN20 | HB3 | 1.00 | 0.011 | 1.00 | 0.10 |
| ASN20 | HD21 | 1.00 | 0.001 | 1.00 | -1089370.00 |
| ASN20 | HD22 | 1.00 | 0.013 | 1.00 | -474376.00 |

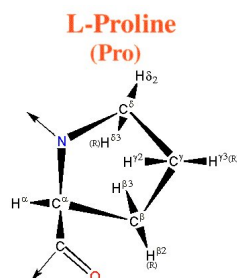
3.21 PRO(21)

Figure 11: Image from the BMRB

Residue probability: 0.810

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 177.473 | 175.173 | 13.901 | 0.000 | 0.000 |
| CA 3.21.1 | 64.513 | 62.931 | 15.301 | 0.811 | 1.000 |
| CB 3.21.2 | 32.124 | 33.632 | 13.629 | 0.889 | 1.000 |
| CG 3.21.3 | 27.140 | 28.412 | 13.801 | 0.714 | 1.000 |
| CD 3.21.4 | 51.083 | 49.797 | 3.175 | 1.000 | 1.000 |
| N | NA | – | – | 0.000 | 0.000 |
| HA 3.21.5 | 4.612 | 4.332 | 0.427 | 0.880 | 1.000 |
| HB2 3.21.6 | 2.018 | 2.099 | 0.501 | 0.778 | 1.000 |
| HB3 3.21.7 | 2.488 | 2.052 | 0.596 | 1.000 | 1.000 |
| HG2 3.21.8 | 2.104 | 1.927 | 0.364 | 0.443 | 1.000 |
| HG3 3.21.9 | 2.019 | 1.907 | 0.417 | 0.667 | 1.000 |
| HD 3.21.10 | 3.987 | 3.640 | 0.682 | 0.920 | 1.000 |

3.21.1 Detailed Probabilities of PRO21CA:

Overall probability: 0.811

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN20 | 1.00 | 1.00 |
| PRO21 | 0.87 | 1.00 |
| ASN22 | 0.55 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| N20HA | 1.00 |
| P21HB2 | 1.00 |
| P21HB3 | 1.00 |
| P21HG2 | 1.00 |
| P21HG3 | 1.00 |
| P21HD2 | 1.00 |
| P21HA | 1.00 |
| N22H | 1.00 |
| N22HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN20 | HA | 1.00 | 0.015 | 1.00 | 0.12 |
| PRO21 | HA | 1.00 | 0.001 | 1.00 | 22.35 |
| PRO21 | HB2 | 1.00 | 0.000 | 1.00 | 1.89 |
| PRO21 | HB3 | 1.00 | 0.007 | 1.00 | 4.04 |
| PRO21 | HG2 | 1.00 | 0.002 | 1.00 | 1.94 |
| PRO21 | HG3 | 1.00 | 0.001 | 1.00 | 1.89 |
| PRO21 | HD2 | 1.00 | 0.038 | 0.20 | 0.00 |
| ASN22 | HA | 1.00 | 0.039 | 0.10 | 0.00 |
| ASN22 | H | 1.00 | 0.014 | 1.00 | 0.38 |

3.21.2 Detailed Probabilities of PRO21CB:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO21 | 0.83 | 1.00 |
| ASN22 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P21HA | 1.00 |
| P21HB3 | 1.00 |
| P21HG2 | 1.00 |
| P21HG3 | 1.00 |
| P21HD2 | 1.00 |
| P21HB2 | 1.00 |
| N22HA | 0.98 |
| N22H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO21 | HA | 1.00 | 0.002 | 1.00 | 1.52 |
| PRO21 | HB2 | 1.00 | 0.000 | 1.00 | 17.43 |
| PRO21 | HB3 | 1.00 | 0.002 | 1.00 | 6.24 |
| PRO21 | HG2 | 1.00 | 0.086 | 0.00 | 0.00 |
| PRO21 | HG3 | 1.00 | 0.001 | 1.00 | 17.43 |
| PRO21 | HD2 | 1.00 | 0.004 | 1.00 | 0.88 |
| ASN22 | HA | 0.98 | 0.007 | 1.00 | 0.16 |
| ASN22 | H | 1.00 | 0.003 | 1.00 | 0.12 |
| ASN22 | HB2 | 0.56 | 0.004 | 1.00 | 0.53 |

3.21.3 Detailed Probabilities of PRO21CG:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN20 | 1.00 | 1.00 |
| PRO21 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| N20HA | 0.95 |
| P21HA | 1.00 |
| P21HB2 | 1.00 |
| P21HB3 | 1.00 |
| P21HG3 | 1.00 |
| P21HD2 | 1.00 |
| P21HG2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN20 | HA | 0.95 | 0.001 | 1.00 | 0.27 |
| PRO21 | HA | 1.00 | 0.003 | 1.00 | 0.60 |
| PRO21 | HB2 | 1.00 | 0.065 | 0.00 | 0.00 |
| PRO21 | HB3 | 1.00 | 0.011 | 1.00 | 2.08 |
| PRO21 | HG2 | 1.00 | 0.021 | 1.00 | 31.34 |
| PRO21 | HG3 | 1.00 | 0.064 | 0.00 | 0.00 |
| PRO21 | HD2 | 1.00 | 0.002 | 1.00 | 1.66 |

3.21.4 Detailed Probabilities of PRO21CD:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN20 | 1.00 | 1.00 |
| PRO21 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| N20HB2 | 0.98 |
| N20HA | 1.00 |
| N20H | 1.00 |
| N20HB3 | 0.98 |
| P21HA | 1.00 |
| P21HB2 | 1.00 |
| P21HB3 | 1.00 |
| P21HG2 | 1.00 |
| P21HG3 | 1.00 |
| P21HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN20 | HA | 1.00 | 0.001 | 1.00 | 1.81 |
| ASN20 | HB2 | 0.98 | 0.000 | 1.00 | 0.10 |
| ASN20 | HB3 | 0.99 | 0.006 | 1.00 | 0.16 |
| ASN20 | H | 0.99 | 0.004 | 1.00 | 0.05 |
| PRO21 | HA | 1.00 | 0.001 | 1.00 | 0.17 |
| PRO21 | HB2 | 1.00 | 0.003 | 1.00 | 1.30 |
| PRO21 | HB3 | 1.00 | 0.001 | 1.00 | 0.30 |
| PRO21 | HG2 | 1.00 | 0.003 | 1.00 | 1.16 |
| PRO21 | HG3 | 1.00 | 0.004 | 1.00 | 1.30 |
| PRO21 | HD2 | 1.00 | 0.004 | 1.00 | 8.06 |

3.21.5 Detailed Probabilities of PRO21HA:

Overall probability: 0.880

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN20 | 0.50 | 1.00 |
| PRO21 | 1.00 | 1.00 |
| ASN22 | 0.90 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| N20HA | 1.00 |
| P21HB2 | 1.00 |
| P21HB3 | 1.00 |
| P21HG2 | 1.00 |
| P21HG3 | 1.00 |
| P21HD2 | 1.00 |
| P21HA | 1.00 |
| N22H | 1.00 |
| N22HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN20 | HA | 1.00 | 0.053 | 0.00 | 0.00 |
| ASN20 | H | 0.76 | 0.006 | 1.00 | -134878.00 |
| PRO21 | HA | 1.00 | 0.001 | 1.00 | 22.35 |
| PRO21 | HB2 | 1.00 | 0.002 | 1.00 | 1.52 |
| PRO21 | HB3 | 1.00 | 0.001 | 1.00 | 2.53 |
| PRO21 | HG2 | 1.00 | 0.003 | 1.00 | 0.60 |
| PRO21 | HG3 | 1.00 | 0.004 | 1.00 | 0.47 |
| PRO21 | HD2 | 1.00 | 0.001 | 1.00 | 0.17 |
| ASN22 | HA | 1.00 | 0.032 | 0.80 | 0.00 |
| ASN22 | H | 1.00 | 0.004 | 1.00 | -312189.00 |

3.21.6 Detailed Probabilities of PRO21HB2:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO21 | 0.67 | 1.00 |
| ASN22 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P21HA | 1.00 |
| P21HB3 | 1.00 |
| P21HG2 | 1.00 |
| P21HG3 | 1.00 |
| P21HD2 | 1.00 |
| P21HB2 | 1.00 |
| N22HA | 0.98 |
| N22H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO21 | HA | 1.00 | 0.000 | 1.00 | 1.89 |
| PRO21 | HB2 | 1.00 | 0.000 | 1.00 | 17.43 |
| PRO21 | HB3 | 1.00 | 0.003 | 1.00 | 8.06 |
| PRO21 | HG2 | 1.00 | 0.065 | 0.00 | 0.00 |
| PRO21 | HG3 | 1.00 | 0.466 | 0.00 | 0.00 |
| PRO21 | HD2 | 1.00 | 0.003 | 1.00 | 1.30 |
| ASN22 | HA | 0.98 | 0.021 | 1.00 | 1.00 |
| ASN22 | H | 1.00 | 0.007 | 1.00 | -524762.00 |
| ASN22 | HB2 | 0.56 | 0.003 | 1.00 | 0.09 |

3.21.7 Detailed Probabilities of PRO21HB3:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO21 | 1.00 | 1.00 |
| ASN22 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P21HA | 1.00 |
| P21HB2 | 1.00 |
| P21HG2 | 1.00 |
| P21HG3 | 1.00 |
| P21HD2 | 1.00 |
| P21HB3 | 1.00 |
| N22H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO21 | HA | 1.00 | 0.007 | 1.00 | 4.04 |
| PRO21 | HB2 | 1.00 | 0.002 | 1.00 | 6.24 |
| PRO21 | HB3 | 1.00 | 0.003 | 1.00 | 12.02 |
| PRO21 | HG2 | 1.00 | 0.011 | 1.00 | 2.08 |
| PRO21 | HG3 | 1.00 | 0.004 | 1.00 | 1.33 |
| PRO21 | HD2 | 1.00 | 0.001 | 1.00 | 0.30 |
| ASN22 | H | 1.00 | 0.005 | 1.00 | -148213.00 |

3.21.8 Detailed Probabilities of PRO21HG2:

Overall probability: 0.443

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN20 | 0.10 | 1.00 |
| PRO21 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| N20HA | 0.95 |
| P21HA | 1.00 |
| P21HB2 | 1.00 |
| P21HB3 | 1.00 |
| P21HG3 | 1.00 |
| P21HD2 | 1.00 |
| P21HG2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN20 | HA | 0.95 | 0.039 | 0.10 | 0.00 |
| PRO21 | HA | 1.00 | 0.002 | 1.00 | 1.94 |
| PRO21 | HB2 | 1.00 | 0.086 | 0.00 | 0.00 |
| PRO21 | HB3 | 1.00 | 0.089 | 0.00 | 0.00 |
| PRO21 | HG2 | 1.00 | 0.021 | 1.00 | 31.34 |
| PRO21 | HG3 | 1.00 | 0.380 | 0.00 | 0.00 |
| PRO21 | HD2 | 1.00 | 0.003 | 1.00 | 1.16 |

3.21.9 Detailed Probabilities of PRO21HG3:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO21 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P21HA | 1.00 |
| P21HB2 | 1.00 |
| P21HB3 | 1.00 |
| P21HG2 | 1.00 |
| P21HD2 | 1.00 |
| P21HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO21 | HA | 1.00 | 0.001 | 1.00 | 1.89 |
| PRO21 | HB2 | 1.00 | 0.001 | 1.00 | 17.43 |
| PRO21 | HB3 | 1.00 | 0.004 | 1.00 | 8.06 |
| PRO21 | HG2 | 1.00 | 0.064 | 0.00 | 0.00 |
| PRO21 | HG3 | 1.00 | 0.465 | 0.00 | 0.00 |
| PRO21 | HD2 | 1.00 | 0.004 | 1.00 | 1.30 |

3.21.10 Detailed Probabilities of PRO21HD2:

Overall probability: 0.920

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN20 | 1.00 | 1.00 |
| PRO21 | 0.87 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| N20HB2 | 0.98 |
| N20HA | 1.00 |
| N20H | 1.00 |
| N20HB3 | 0.98 |
| P21HA | 1.00 |
| P21HB2 | 1.00 |
| P21HB3 | 1.00 |
| P21HG2 | 1.00 |
| P21HG3 | 1.00 |
| P21HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN20 | HA | 1.00 | 0.001 | 1.00 | 3.00 |
| ASN20 | HB2 | 0.98 | 0.003 | 1.00 | 0.22 |
| ASN20 | HB3 | 0.99 | 0.010 | 1.00 | 0.48 |
| ASN20 | H | 0.99 | 0.001 | 1.00 | -282499.00 |
| PRO21 | HA | 1.00 | 0.038 | 0.20 | 0.00 |
| PRO21 | HB2 | 1.00 | 0.004 | 1.00 | 0.88 |
| PRO21 | HB3 | 1.00 | 0.001 | 1.00 | 0.67 |
| PRO21 | HG2 | 1.00 | 0.002 | 1.00 | 1.66 |
| PRO21 | HG3 | 1.00 | 0.001 | 1.00 | 1.55 |
| PRO21 | HD2 | 1.00 | 0.004 | 1.00 | 8.06 |

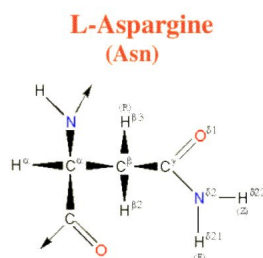
3.22 ASN(22)

Figure 12: Image from the BMRB

Residue probability: 0.834

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|--------------|-------------|---------|--------|---------------------|--------------------|
| C | 174.014 | 175.315 | 1.862 | 0.000 | 0.000 |
| CA 3.22.1 | 53.492 | 53.674 | 5.429 | 0.680 | 1.000 |
| CB 3.22.2 | 38.310 | 38.785 | 5.449 | 0.857 | 1.000 |
| N 3.22.3 | 113.190 | 118.907 | 6.480 | 1.000 | 1.000 |
| ND2 3.22.4 | 110.325 | 112.932 | 14.355 | 1.000 | 1.000 |
| HA 3.22.5 | 4.881 | 4.658 | 0.371 | 0.736 | 1.000 |
| HB2 3.22.6 | 3.166 | 2.800 | 0.341 | 1.000 | 1.000 |
| HB3 3.22.7 | 2.736 | 2.739 | 0.364 | 0.571 | 1.000 |
| H 3.22.8 | 8.439 | 8.328 | 0.633 | 1.000 | 1.000 |
| HD21 3.22.9 | 7.270 | 7.343 | 1.188 | 0.667 | 1.000 |
| HD22 3.22.10 | 6.280 | 7.145 | 1.184 | 0.833 | 1.000 |

3.22.1 Detailed Probabilities of ASN22CA:

Overall probability: 0.680

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO21 | 0.90 | 1.00 |
| ASN22 | 0.50 | 1.00 |
| SER23 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P21HB2 | 0.98 |
| P21HA | 1.00 |
| N22HB2 | 1.00 |
| N22HB3 | 1.00 |
| N22H | 1.00 |
| N22HD21 | 1.00 |
| N22HD22 | 1.00 |
| N22HA | 1.00 |
| S23H | 1.00 |
| S23HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO21 | HA | 1.00 | 0.032 | 0.80 | 0.00 |
| PRO21 | HB2 | 0.98 | 0.021 | 1.00 | 1.00 |
| ASN22 | HA | 1.00 | 0.007 | 1.00 | 4.15 |
| ASN22 | HB2 | 1.00 | 0.010 | 1.00 | 0.33 |
| ASN22 | HB3 | 1.00 | 0.045 | 0.00 | 0.00 |
| ASN22 | H | 1.00 | 0.020 | 1.00 | 0.65 |
| ASN22 | HD21 | 1.00 | 0.106 | 0.00 | 0.00 |
| ASN22 | HD22 | 1.00 | 0.065 | 0.00 | 0.00 |
| SER23 | HA | 1.00 | 0.014 | 1.00 | 0.99 |
| SER23 | H | 1.00 | 0.000 | 1.00 | 0.84 |

3.22.2 Detailed Probabilities of ASN22CB:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN22 | 0.83 | 1.00 |
| SER23 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N22HA | 1.00 |
| N22HB2 | 1.00 |
| N22H | 1.00 |
| N22HD21 | 1.00 |
| N22HD22 | 1.00 |
| N22HB3 | 1.00 |
| S23H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN22 | HA | 1.00 | 0.003 | 1.00 | 0.35 |
| ASN22 | HB2 | 1.00 | 0.004 | 1.00 | 1.90 |
| ASN22 | HB3 | 1.00 | 0.389 | 0.00 | 0.00 |
| ASN22 | H | 1.00 | 0.002 | 1.00 | 0.22 |
| ASN22 | HD21 | 1.00 | 0.003 | 1.00 | 0.40 |
| ASN22 | HD22 | 1.00 | 0.000 | 1.00 | 0.24 |
| SER23 | H | 1.00 | 0.001 | 1.00 | 0.08 |

3.22.3 Detailed Probabilities of ASN22N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO21 | 1.00 | 1.00 |
| ASN22 | 1.00 | 1.00 |
| SER23 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P21HB2 | 1.00 |
| P21HA | 1.00 |
| P21HB3 | 1.00 |
| N22HA | 1.00 |
| N22HB2 | 1.00 |
| N22HB3 | 1.00 |
| N22HD21 | 0.98 |
| N22H | 1.00 |
| S23H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO21 | HA | 1.00 | 0.004 | 1.00 | -312189.00 |
| PRO21 | HB2 | 1.00 | 0.007 | 1.00 | -524762.00 |
| PRO21 | HB3 | 1.00 | 0.005 | 1.00 | -148213.00 |
| PRO21 | HG2 | 0.95 | 0.009 | 1.00 | -113081.00 |
| PRO21 | HG3 | 0.84 | 0.008 | 1.00 | -524762.00 |
| PRO21 | HD2 | 0.77 | 0.003 | 1.00 | -349089.00 |
| ASN22 | HA | 1.00 | 0.008 | 1.00 | -343355.00 |
| ASN22 | HB2 | 1.00 | 0.008 | 1.00 | -329614.00 |
| ASN22 | HB3 | 1.00 | 0.002 | 1.00 | -472338.00 |
| ASN22 | H | 1.00 | 0.002 | 1.00 | -2181710.00 |
| ASN22 | HD21 | 0.98 | 0.012 | 1.00 | -161760.00 |
| ASN22 | HD22 | 0.63 | 0.008 | 1.00 | -89346.00 |
| SER23 | H | 1.00 | 0.002 | 1.00 | -583733.00 |

3.22.4 Detailed Probabilities of ASN22ND2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN22 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N22HA | 1.00 |
| N22HB2 | 1.00 |
| N22HB3 | 1.00 |
| N22H | 0.98 |
| N22HD22 | 1.00 |
| N22HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN22 | HA | 1.00 | 0.011 | 1.00 | -133838.00 |
| ASN22 | HB2 | 1.00 | 0.006 | 1.00 | -371460.00 |
| ASN22 | HB3 | 1.00 | 0.002 | 1.00 | -437545.00 |
| ASN22 | H | 0.98 | 0.001 | 1.00 | -91068.00 |
| ASN22 | HD21 | 1.00 | 0.002 | 1.00 | -3885305.00 |
| ASN22 | HD22 | 1.00 | 0.002 | 1.00 | -3893872.00 |

3.22.5 Detailed Probabilities of ASN22HA:

Overall probability: 0.736

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO21 | 0.70 | 1.00 |
| ASN22 | 0.83 | 1.00 |
| SER23 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P21HB2 | 0.98 |
| P21HA | 1.00 |
| N22HB2 | 1.00 |
| N22HB3 | 1.00 |
| N22H | 1.00 |
| N22HD21 | 1.00 |
| N22HD22 | 1.00 |
| N22HA | 1.00 |
| S23H | 1.00 |
| S23HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO21 | HA | 1.00 | 0.039 | 0.10 | 0.00 |
| PRO21 | HB2 | 0.98 | 0.007 | 1.00 | 0.16 |
| PRO21 | HG2 | 0.65 | 0.028 | 1.00 | 0.26 |
| ASN22 | HA | 1.00 | 0.007 | 1.00 | 4.15 |
| ASN22 | HB2 | 1.00 | 0.005 | 1.00 | 0.42 |
| ASN22 | HB3 | 1.00 | 0.003 | 1.00 | 0.35 |
| ASN22 | H | 1.00 | 0.008 | 1.00 | -343355.00 |
| ASN22 | HD21 | 1.00 | 0.011 | 1.00 | -133838.00 |
| ASN22 | HD22 | 1.00 | 0.080 | 0.00 | 0.00 |
| SER23 | HA | 1.00 | 0.083 | 0.00 | 0.00 |
| SER23 | H | 1.00 | 0.004 | 1.00 | -279195.00 |

3.22.6 Detailed Probabilities of ASN22HB2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN22 | 1.00 | 1.00 |
| SER23 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N22HA | 1.00 |
| N22HB3 | 1.00 |
| N22H | 1.00 |
| N22HD21 | 1.00 |
| N22HD22 | 1.00 |
| N22HB2 | 1.00 |
| S23H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN22 | HA | 1.00 | 0.010 | 1.00 | 0.33 |
| ASN22 | HB2 | 1.00 | 0.004 | 1.00 | 5.26 |
| ASN22 | HB3 | 1.00 | 0.004 | 1.00 | 1.90 |
| ASN22 | H | 1.00 | 0.008 | 1.00 | -329614.00 |
| ASN22 | HD21 | 1.00 | 0.006 | 1.00 | -371460.00 |
| ASN22 | HD22 | 1.00 | 0.008 | 1.00 | -306374.00 |
| SER23 | H | 1.00 | 0.005 | 1.00 | -86030.00 |

3.22.7 Detailed Probabilities of ASN22HB3:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN22 | 0.67 | 1.00 |
| SER23 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N22HA | 1.00 |
| N22HB2 | 1.00 |
| N22H | 1.00 |
| N22HD21 | 1.00 |
| N22HD22 | 1.00 |
| N22HB3 | 1.00 |
| S23H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN22 | HA | 1.00 | 0.045 | 0.00 | 0.00 |
| ASN22 | HB2 | 1.00 | 0.001 | 1.00 | 1.82 |
| ASN22 | HB3 | 1.00 | 0.389 | 0.00 | 0.00 |
| ASN22 | H | 1.00 | 0.002 | 1.00 | -472338.00 |
| ASN22 | HD21 | 1.00 | 0.002 | 1.00 | -437545.00 |
| ASN22 | HD22 | 1.00 | 0.002 | 1.00 | -426177.00 |
| SER23 | H | 1.00 | 0.046 | 0.00 | 0.00 |

3.22.8 Detailed Probabilities of ASN22H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO21 | 1.00 | 1.00 |
| ASN22 | 1.00 | 1.00 |
| SER23 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P21HB2 | 1.00 |
| P21HA | 1.00 |
| P21HB3 | 1.00 |
| N22HA | 1.00 |
| N22HB2 | 1.00 |
| N22HB3 | 1.00 |
| N22HD21 | 0.98 |
| N22H | 1.00 |
| S23H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO21 | HA | 1.00 | 0.014 | 1.00 | 0.38 |
| PRO21 | HB2 | 1.00 | 0.003 | 1.00 | 0.12 |
| PRO21 | HB3 | 1.00 | 0.004 | 1.00 | 0.11 |
| PRO21 | HG2 | 0.95 | 0.003 | 1.00 | 0.10 |
| PRO21 | HG3 | 0.84 | 0.002 | 1.00 | 0.16 |
| PRO21 | HD2 | 0.77 | 0.014 | 1.00 | 0.09 |
| ASN22 | HA | 1.00 | 0.020 | 1.00 | 0.65 |
| ASN22 | HB2 | 1.00 | 0.005 | 1.00 | 0.18 |
| ASN22 | HB3 | 1.00 | 0.002 | 1.00 | 0.22 |
| ASN22 | H | 1.00 | 0.002 | 1.00 | -2181710.00 |
| ASN22 | HD21 | 0.98 | 0.001 | 1.00 | -91068.00 |
| SER23 | H | 1.00 | 0.008 | 1.00 | -606117.00 |

3.22.9 Detailed Probabilities of ASN22HD21:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN22 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N22HA | 1.00 |
| N22HB2 | 1.00 |
| N22HB3 | 1.00 |
| N22H | 0.98 |
| N22HD22 | 1.00 |
| N22HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN22 | HA | 1.00 | 0.106 | 0.00 | 0.00 |
| ASN22 | HB2 | 1.00 | 0.303 | 0.00 | 0.00 |
| ASN22 | HB3 | 1.00 | 0.003 | 1.00 | 0.40 |
| ASN22 | H | 0.98 | 0.012 | 1.00 | -161760.00 |
| ASN22 | HD21 | 1.00 | 0.002 | 1.00 | -3885305.00 |
| ASN22 | HD22 | 1.00 | 0.002 | 1.00 | -3664250.00 |

3.22.10 Detailed Probabilities of ASN22HD22:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN22 | 0.83 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N22HA | 1.00 |
| N22HB2 | 1.00 |
| N22HB3 | 1.00 |
| N22HD21 | 1.00 |
| N22HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN22 | HA | 1.00 | 0.065 | 0.00 | 0.00 |
| ASN22 | HB2 | 1.00 | 0.003 | 1.00 | 0.16 |
| ASN22 | HB3 | 1.00 | 0.000 | 1.00 | 0.24 |
| ASN22 | HD21 | 1.00 | 0.002 | 1.00 | -3893872.00 |
| ASN22 | HD22 | 1.00 | 0.002 | 1.00 | -4276915.00 |
| ASN22 | H | 0.63 | 0.008 | 1.00 | -89346.00 |

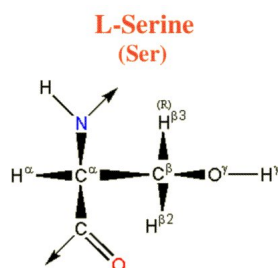
3.23 SER(23)

Figure 13: Image from the BMRB

Residue probability: 0.927

Residue probability confidence: 0.864

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 171.830 | 174.682 | 1.868 | 0.000 | 0.000 |
| CA 3.23.1 | 57.838 | 58.750 | 3.025 | 0.875 | 0.875 |
| CB 3.23.2 | 65.256 | 63.523 | 4.288 | 1.000 | 0.833 |
| N 3.23.3 | 116.802 | 116.135 | 5.326 | 0.889 | 0.900 |
| HA 3.23.4 | 6.167 | 4.486 | 0.430 | 1.000 | 0.875 |
| HB2 3.23.5 | 3.737 | 3.856 | 0.325 | 1.000 | 0.833 |
| HB3 3.23.6 | 3.624 | 3.825 | 0.343 | 0.833 | 0.833 |
| H 3.23.7 | 8.555 | 8.292 | 0.600 | 0.889 | 0.900 |
| HG | NA | – | – | 0.000 | 0.000 |

3.23.1 Detailed Probabilities of SER23CA:

Overall probability: 0.875

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN22 | 0.00 | 1.00 |
| SER23 | 1.00 | 0.80 |
| LEU24 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| N22HA | 1.00 |
| S23HB2 | 1.00 |
| S23HB3 | 1.00 |
| S23H | 1.00 |
| S23HG | 1.00 |
| S23HA | 1.00 |
| L24H | 1.00 |
| L24HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN22 | HA | 1.00 | 0.083 | 0.00 | 0.00 |
| SER23 | HA | 1.00 | 0.002 | 1.00 | 2.07 |
| SER23 | HB2 | 1.00 | 0.006 | 1.00 | 0.26 |
| SER23 | HB3 | 1.00 | 0.002 | 1.00 | 0.41 |
| SER23 | H | 1.00 | 0.002 | 1.00 | 0.15 |
| LEU24 | HA | 1.00 | 0.009 | 1.00 | 0.06 |
| LEU24 | H | 1.00 | 0.006 | 1.00 | 1.08 |
| LEU24 | HB2 | 0.51 | 0.009 | 1.00 | 0.07 |

3.23.2 Detailed Probabilities of SER23CB:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER23 | 1.00 | 0.80 |
| LEU24 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S23HA | 1.00 |
| S23HB3 | 1.00 |
| S23H | 1.00 |
| S23HG | 1.00 |
| S23HB2 | 1.00 |
| L24H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER23 | HA | 1.00 | 0.002 | 1.00 | 0.32 |
| SER23 | HB2 | 1.00 | 0.005 | 1.00 | 3.24 |
| SER23 | HB3 | 1.00 | 0.003 | 1.00 | 3.32 |
| SER23 | H | 1.00 | 0.001 | 1.00 | 0.32 |
| LEU24 | H | 1.00 | 0.007 | 1.00 | 0.21 |
| LEU24 | HA | 0.68 | 0.013 | 1.00 | 0.06 |

3.23.3 Detailed Probabilities of SER23N:

Overall probability: 0.889

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN22 | 0.75 | 1.00 |
| SER23 | 1.00 | 0.80 |
| LEU24 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| N22HA | 1.00 |
| N22H | 1.00 |
| N22HB2 | 1.00 |
| N22HB3 | 1.00 |
| S23HA | 1.00 |
| S23HB2 | 1.00 |
| S23HB3 | 1.00 |
| S23HG | 1.00 |
| S23H | 1.00 |
| L24H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN22 | HA | 1.00 | 0.004 | 1.00 | -279195.00 |
| ASN22 | HB2 | 1.00 | 0.005 | 1.00 | -86030.00 |
| ASN22 | HB3 | 1.00 | 0.046 | 0.00 | 0.00 |
| ASN22 | H | 1.00 | 0.008 | 1.00 | -606117.00 |
| SER23 | HA | 1.00 | 0.000 | 1.00 | -454605.00 |
| SER23 | HB2 | 1.00 | 0.006 | 1.00 | -732150.00 |
| SER23 | HB3 | 1.00 | 0.002 | 1.00 | -472475.00 |
| SER23 | H | 1.00 | 0.001 | 1.00 | -8389601.00 |
| LEU24 | H | 1.00 | 0.007 | 1.00 | -240481.00 |

3.23.4 Detailed Probabilities of SER23HA:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN22 | 1.00 | 1.00 |
| SER23 | 1.00 | 0.80 |
| LEU24 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| N22HA | 1.00 |
| S23HB2 | 1.00 |
| S23HB3 | 1.00 |
| S23H | 1.00 |
| S23HG | 1.00 |
| S23HA | 1.00 |
| L24H | 1.00 |
| L24HA | 1.00 |

NOESY contacts detailed probability

3.23 SER(23)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN22 | HA | 1.00 | 0.014 | 1.00 | 0.99 |
| SER23 | HA | 1.00 | 0.002 | 1.00 | 2.07 |
| SER23 | HB2 | 1.00 | 0.002 | 1.00 | 0.32 |
| SER23 | HB3 | 1.00 | 0.002 | 1.00 | 0.43 |
| SER23 | H | 1.00 | 0.000 | 1.00 | -454605.00 |
| LEU24 | HA | 1.00 | 0.005 | 1.00 | 0.09 |
| LEU24 | H | 1.00 | 0.003 | 1.00 | -2036674.00 |
| LEU24 | HB2 | 0.51 | 0.003 | 1.00 | 0.07 |

3.23.5 Detailed Probabilities of SER23HB2:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER23 | 1.00 | 0.80 |
| LEU24 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S23HA | 1.00 |
| S23HB3 | 1.00 |
| S23H | 1.00 |
| S23HG | 1.00 |
| S23HB2 | 1.00 |
| L24H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER23 | HA | 1.00 | 0.006 | 1.00 | 0.26 |
| SER23 | HB2 | 1.00 | 0.005 | 1.00 | 3.24 |
| SER23 | HB3 | 1.00 | 0.002 | 1.00 | 2.73 |
| SER23 | H | 1.00 | 0.006 | 1.00 | -732150.00 |
| LEU24 | H | 1.00 | 0.009 | 1.00 | -312295.00 |

3.23.6 Detailed Probabilities of SER23HB3:

Overall probability: 0.833

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER23 | 0.75 | 0.80 |
| LEU24 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S23HA | 1.00 |
| S23HB2 | 1.00 |
| S23H | 1.00 |
| S23HG | 1.00 |
| S23HB3 | 1.00 |
| L24H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER23 | HA | 1.00 | 0.002 | 1.00 | 0.41 |
| SER23 | HB2 | 1.00 | 0.003 | 1.00 | 3.32 |
| SER23 | HB3 | 1.00 | 0.073 | 0.00 | 0.00 |
| SER23 | H | 1.00 | 0.002 | 1.00 | -472475.00 |
| LEU24 | H | 1.00 | 0.002 | 1.00 | -565080.00 |
| LEU24 | HA | 0.76 | 0.002 | 1.00 | 0.10 |

3.23.7 Detailed Probabilities of SER23H:

Overall probability: 0.889

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN22 | 0.75 | 1.00 |
| SER23 | 1.00 | 0.80 |
| LEU24 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| N22HA | 1.00 |
| N22H | 1.00 |
| N22HB2 | 1.00 |
| N22HB3 | 1.00 |
| S23HA | 1.00 |
| S23HB2 | 1.00 |
| S23HB3 | 1.00 |
| S23HG | 1.00 |
| S23H | 1.00 |
| L24H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN22 | HA | 1.00 | 0.000 | 1.00 | 0.84 |
| ASN22 | HB2 | 1.00 | 0.076 | 0.00 | 0.00 |
| ASN22 | HB3 | 1.00 | 0.001 | 1.00 | 0.08 |
| ASN22 | H | 1.00 | 0.002 | 1.00 | -583733.00 |
| SER23 | HA | 1.00 | 0.002 | 1.00 | 0.15 |
| SER23 | HB2 | 1.00 | 0.001 | 1.00 | 0.32 |
| SER23 | HB3 | 1.00 | 0.002 | 1.00 | 0.24 |
| SER23 | H | 1.00 | 0.001 | 1.00 | -8389601.00 |
| LEU24 | H | 1.00 | 0.009 | 1.00 | -118114.00 |

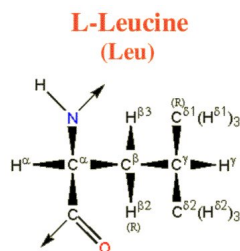
3.24 LEU(24)

Figure 14: Image from the BMRB

Residue probability: 0.834

Residue probability confidence: 0.986

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 173.520 | 177.056 | 1.929 | 0.000 | 0.000 |
| CA 3.24.1 | 53.734 | 55.735 | 3.802 | 0.637 | 1.000 |
| CB 3.24.2 | 45.982 | 42.389 | 3.750 | 1.000 | 1.000 |
| CG 3.24.3 | 25.790 | 26.892 | 3.086 | 0.887 | 1.000 |
| CD1 3.24.4 | 23.238 | 24.837 | 3.657 | 0.857 | 1.000 |
| CD2 3.24.5 | 24.100 | 24.201 | 3.117 | 0.714 | 1.000 |
| N 3.24.6 | 126.813 | 121.785 | 4.943 | 1.000 | 0.909 |
| HA 3.24.7 | 4.462 | 4.315 | 0.840 | 0.818 | 1.000 |
| HB2 3.24.8 | 0.413 | 1.601 | 0.373 | 1.000 | 1.000 |
| HB3 3.24.9 | 0.174 | 1.508 | 0.398 | 0.875 | 1.000 |
| HG 3.24.10 | 0.407 | 1.510 | 0.340 | 1.000 | 1.000 |
| HD1 3.24.11 | -0.029 | 0.739 | 0.294 | 0.857 | 1.000 |
| HD2 3.24.12 | 0.029 | 0.727 | 0.421 | 0.351 | 1.000 |
| H 3.24.13 | 8.732 | 8.237 | 0.647 | 0.842 | 0.909 |

3.24.1 Detailed Probabilities of LEU24CA:

Overall probability: 0.637

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER23 | 1.00 | 1.00 |
| LEU24 | 0.57 | 1.00 |
| LYS25 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| S23HA | 1.00 |
| L24HB2 | 1.00 |
| L24HB3 | 1.00 |
| L24HG | 1.00 |
| L24HD11 | 0.99 |
| L24HD21 | 0.99 |
| L24H | 1.00 |
| L24HA | 1.00 |
| K25HA | 1.00 |
| K25H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER23 | HA | 1.00 | 0.005 | 1.00 | 0.09 |
| SER23 | HB3 | 0.76 | 0.002 | 1.00 | 0.10 |
| LEU24 | HA | 1.00 | 0.152 | 0.00 | 0.00 |
| LEU24 | HB2 | 1.00 | 0.004 | 1.00 | 0.61 |
| LEU24 | HB3 | 1.00 | 0.014 | 1.00 | 0.42 |
| LEU24 | HG | 1.00 | 0.002 | 1.00 | 0.61 |
| LEU24 | HD11 | 0.99 | 0.015 | 1.00 | 0.84 |
| LEU24 | HD21 | 0.99 | 0.043 | 0.01 | 0.00 |
| LEU24 | H | 1.00 | 0.131 | 0.00 | 0.00 |
| LYS25 | HA | 1.00 | 0.104 | 0.00 | 0.00 |
| LYS25 | H | 1.00 | 0.009 | 1.00 | 1.10 |

3.24.2 Detailed Probabilities of LEU24CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU24 | 1.00 | 1.00 |
| LYS25 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L24HA | 1.00 |
| L24HB3 | 1.00 |
| L24HG | 1.00 |
| L24HD11 | 1.00 |
| L24HD21 | 1.00 |
| L24H | 1.00 |
| L24HB2 | 1.00 |
| K25H | 1.00 |

NOESY contacts detailed probability

3.24 LEU(24)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU24 | HA | 1.00 | 0.000 | 1.00 | 0.42 |
| LEU24 | HB2 | 1.00 | 0.005 | 1.00 | 4.14 |
| LEU24 | HB3 | 1.00 | 0.007 | 1.00 | 2.02 |
| LEU24 | HG | 1.00 | 0.001 | 1.00 | 4.14 |
| LEU24 | HD11 | 1.00 | 0.029 | 1.00 | 0.96 |
| LEU24 | HD21 | 1.00 | 0.029 | 1.00 | 0.96 |
| LEU24 | H | 1.00 | 0.008 | 1.00 | 0.32 |
| LYS25 | H | 1.00 | 0.007 | 1.00 | 0.20 |

3.24.3 Detailed Probabilities of LEU24CG:

Overall probability: 0.887

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU24 | 0.87 | 1.00 |
| LYS25 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L24HA | 1.00 |
| L24HB2 | 1.00 |
| L24HB3 | 1.00 |
| L24HD11 | 1.00 |
| L24HD21 | 1.00 |
| L24H | 1.00 |
| L24HG | 1.00 |
| K25H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU24 | HA | 1.00 | 0.002 | 1.00 | 0.24 |
| LEU24 | HB2 | 1.00 | 0.007 | 1.00 | 5.08 |
| LEU24 | HB3 | 1.00 | 0.003 | 1.00 | 0.58 |
| LEU24 | HG | 1.00 | 0.001 | 1.00 | 5.08 |
| LEU24 | HD11 | 1.00 | 0.019 | 1.00 | 0.96 |
| LEU24 | HD21 | 1.00 | 0.039 | 0.10 | 0.00 |
| LEU24 | H | 1.00 | 0.017 | 1.00 | 0.14 |
| LYS25 | H | 0.98 | 0.006 | 1.00 | 0.18 |

3.24.4 Detailed Probabilities of LEU24CD1:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU24 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L24HA | 0.99 |
| L24HB2 | 1.00 |
| L24HB3 | 1.00 |
| L24HG | 1.00 |
| L24HD12 | 1.00 |
| L24HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU24 | HA | 0.99 | 0.002 | 1.00 | 1.12 |
| LEU24 | HB2 | 1.00 | 0.009 | 1.00 | 2.04 |
| LEU24 | HB3 | 1.00 | 0.004 | 1.00 | 0.70 |
| LEU24 | HG | 1.00 | 0.003 | 1.00 | 2.04 |
| LEU24 | HD11 | 1.00 | 0.007 | 1.00 | 54.52 |
| LEU24 | HD21 | 1.00 | 0.065 | 0.00 | 0.00 |
| LEU24 | H | 0.86 | 0.025 | 1.00 | 0.33 |

3.24.5 Detailed Probabilities of LEU24CD2:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU24 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L24HA | 0.99 |
| L24HB2 | 1.00 |
| L24HB3 | 1.00 |
| L24HG | 1.00 |
| L24HD11 | 1.00 |
| L24HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU24 | HA | 0.99 | 0.001 | 1.00 | 0.72 |
| LEU24 | HB2 | 1.00 | 0.007 | 1.00 | 2.10 |
| LEU24 | HB3 | 1.00 | 0.047 | 0.00 | 0.00 |
| LEU24 | HG | 1.00 | 0.001 | 1.00 | 2.10 |
| LEU24 | HD11 | 1.00 | 0.047 | 0.00 | 0.00 |
| LEU24 | HD21 | 1.00 | 0.011 | 1.00 | 50.33 |
| LEU24 | H | 0.85 | 0.016 | 1.00 | 0.25 |

3.24.6 Detailed Probabilities of LEU24N:

Overall probability: 1.000

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER23 | 1.00 | 0.80 |
| LEU24 | 1.00 | 1.00 |
| LYS25 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S23HG | 0.97 |
| S23HB3 | 1.00 |
| S23H | 1.00 |
| S23HB2 | 1.00 |
| S23HA | 1.00 |
| L24HA | 1.00 |
| L24HB2 | 1.00 |
| L24HB3 | 1.00 |
| L24HG | 1.00 |
| L24H | 1.00 |
| K25H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER23 | HA | 1.00 | 0.003 | 1.00 | -2036674.00 |
| SER23 | HB2 | 1.00 | 0.009 | 1.00 | -312295.00 |
| SER23 | HB3 | 1.00 | 0.002 | 1.00 | -565080.00 |
| SER23 | H | 1.00 | 0.009 | 1.00 | -118114.00 |
| LEU24 | HA | 1.00 | 0.000 | 1.00 | -568072.00 |
| LEU24 | HB2 | 1.00 | 0.004 | 1.00 | -788611.00 |
| LEU24 | HB3 | 1.00 | 0.007 | 1.00 | -602561.00 |
| LEU24 | HG | 1.00 | 0.002 | 1.00 | -788611.00 |
| LEU24 | H | 1.00 | 0.004 | 1.00 | -8900762.00 |
| LEU24 | HD11 | 0.88 | 0.017 | 1.00 | -277555.00 |
| LYS25 | H | 1.00 | 0.011 | 1.00 | -126929.00 |
| LYS25 | HA | 0.89 | 0.007 | 1.00 | -111239.00 |

3.24.7 Detailed Probabilities of LEU24HA:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER23 | 1.00 | 1.00 |
| LEU24 | 0.86 | 1.00 |
| LYS25 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| S23HA | 1.00 |
| L24HB2 | 1.00 |
| L24HB3 | 1.00 |
| L24HG | 1.00 |
| L24HD11 | 0.99 |
| L24HD21 | 0.99 |
| L24H | 1.00 |
| L24HA | 1.00 |
| K25HA | 1.00 |
| K25H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER23 | HA | 1.00 | 0.009 | 1.00 | 0.06 |
| SER23 | HB2 | 0.68 | 0.013 | 1.00 | 0.06 |
| LEU24 | HA | 1.00 | 0.152 | 0.00 | 0.00 |
| LEU24 | HB2 | 1.00 | 0.000 | 1.00 | 0.42 |
| LEU24 | HB3 | 1.00 | 0.001 | 1.00 | 0.41 |
| LEU24 | HG | 1.00 | 0.002 | 1.00 | 0.24 |
| LEU24 | HD11 | 0.99 | 0.002 | 1.00 | 1.12 |
| LEU24 | HD21 | 0.99 | 0.001 | 1.00 | 0.72 |
| LEU24 | H | 1.00 | 0.000 | 1.00 | -568072.00 |
| LYS25 | HA | 1.00 | 0.400 | 0.00 | 0.00 |
| LYS25 | H | 1.00 | 0.000 | 1.00 | -1954649.00 |

3.24.8 Detailed Probabilities of LEU24HB2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU24 | 1.00 | 1.00 |
| LYS25 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L24HA | 1.00 |
| L24HB3 | 1.00 |
| L24HG | 1.00 |
| L24HD11 | 1.00 |
| L24HD21 | 1.00 |
| L24H | 1.00 |
| L24HB2 | 1.00 |
| K25H | 1.00 |

NOESY contacts detailed probability

3.24 LEU(24)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU24 | HA | 1.00 | 0.004 | 1.00 | 0.61 |
| LEU24 | HB2 | 1.00 | 0.005 | 1.00 | 4.14 |
| LEU24 | HB3 | 1.00 | 0.006 | 1.00 | 2.71 |
| LEU24 | HG | 1.00 | 0.007 | 1.00 | 5.08 |
| LEU24 | HD11 | 1.00 | 0.009 | 1.00 | 2.04 |
| LEU24 | HD21 | 1.00 | 0.007 | 1.00 | 2.10 |
| LEU24 | H | 1.00 | 0.004 | 1.00 | -788611.00 |
| LYS25 | H | 1.00 | 0.006 | 1.00 | -632202.00 |

3.24.9 Detailed Probabilities of LEU24HB3:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU24 | 0.86 | 1.00 |
| LYS25 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L24HA | 1.00 |
| L24HB2 | 1.00 |
| L24HG | 1.00 |
| L24HD11 | 1.00 |
| L24HD21 | 1.00 |
| L24H | 1.00 |
| L24HB3 | 1.00 |
| K25H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU24 | HA | 1.00 | 0.014 | 1.00 | 0.42 |
| LEU24 | HB2 | 1.00 | 0.007 | 1.00 | 2.02 |
| LEU24 | HB3 | 1.00 | 0.006 | 1.00 | 2.79 |
| LEU24 | HG | 1.00 | 0.003 | 1.00 | 0.58 |
| LEU24 | HD11 | 1.00 | 0.004 | 1.00 | 0.70 |
| LEU24 | HD21 | 1.00 | 0.047 | 0.00 | 0.00 |
| LEU24 | H | 1.00 | 0.007 | 1.00 | -602561.00 |
| LYS25 | H | 1.00 | 0.002 | 1.00 | -179511.00 |

3.24.10 Detailed Probabilities of LEU24HG:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU24 | 1.00 | 1.00 |
| LYS25 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L24HA | 1.00 |
| L24HB2 | 1.00 |
| L24HB3 | 1.00 |
| L24HD11 | 1.00 |
| L24HD21 | 1.00 |
| L24H | 1.00 |
| L24HG | 1.00 |
| K25H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU24 | HA | 1.00 | 0.002 | 1.00 | 0.61 |
| LEU24 | HB2 | 1.00 | 0.001 | 1.00 | 4.14 |
| LEU24 | HB3 | 1.00 | 0.000 | 1.00 | 2.71 |
| LEU24 | HG | 1.00 | 0.001 | 1.00 | 5.08 |
| LEU24 | HD11 | 1.00 | 0.003 | 1.00 | 2.04 |
| LEU24 | HD21 | 1.00 | 0.001 | 1.00 | 2.10 |
| LEU24 | H | 1.00 | 0.002 | 1.00 | -788611.00 |
| LYS25 | H | 0.98 | 0.000 | 1.00 | -632202.00 |

3.24.11 Detailed Probabilities of LEU24HD11:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU24 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L24HA | 0.99 |
| L24HB2 | 1.00 |
| L24HB3 | 1.00 |
| L24HG | 1.00 |
| L24HD12 | 1.00 |
| L24HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU24 | HA | 0.99 | 0.015 | 1.00 | 0.84 |
| LEU24 | HB2 | 1.00 | 0.029 | 1.00 | 0.96 |
| LEU24 | HB3 | 1.00 | 0.014 | 1.00 | 0.90 |
| LEU24 | HG | 1.00 | 0.019 | 1.00 | 0.96 |
| LEU24 | HD11 | 1.00 | 0.007 | 1.00 | 54.52 |
| LEU24 | HD21 | 1.00 | 0.047 | 0.00 | 0.00 |
| LEU24 | H | 0.86 | 0.017 | 1.00 | -277555.00 |

3.24.12 Detailed Probabilities of LEU24HD21:

Overall probability: 0.351

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU24 | 0.35 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L24HA | 0.99 |
| L24HB2 | 1.00 |
| L24HB3 | 1.00 |
| L24HG | 1.00 |
| L24HD11 | 1.00 |
| L24HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU24 | HA | 0.99 | 0.043 | 0.01 | 0.00 |
| LEU24 | HB2 | 1.00 | 0.029 | 1.00 | 0.96 |
| LEU24 | HB3 | 1.00 | 0.044 | 0.00 | 0.00 |
| LEU24 | HG | 1.00 | 0.039 | 0.10 | 0.00 |
| LEU24 | HD11 | 1.00 | 0.065 | 0.00 | 0.00 |
| LEU24 | HD21 | 1.00 | 0.011 | 1.00 | 50.33 |

3.24.13 Detailed Probabilities of LEU24H:

Overall probability: 0.842

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER23 | 1.00 | 0.80 |
| LEU24 | 0.86 | 1.00 |
| LYS25 | 0.10 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S23HG | 0.97 |
| S23HB3 | 1.00 |
| S23H | 1.00 |
| S23HB2 | 1.00 |
| S23HA | 1.00 |
| L24HA | 1.00 |
| L24HB2 | 1.00 |
| L24HB3 | 1.00 |
| L24HG | 1.00 |
| L24H | 1.00 |
| K25H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER23 | HA | 1.00 | 0.006 | 1.00 | 1.08 |
| SER23 | HB2 | 1.00 | 0.007 | 1.00 | 0.21 |
| SER23 | HB3 | 1.00 | 0.007 | 1.00 | 0.27 |
| SER23 | H | 1.00 | 0.007 | 1.00 | -240481.00 |
| LEU24 | HA | 1.00 | 0.131 | 0.00 | 0.00 |
| LEU24 | HB2 | 1.00 | 0.008 | 1.00 | 0.32 |
| LEU24 | HB3 | 1.00 | 0.009 | 1.00 | 0.31 |
| LEU24 | HG | 1.00 | 0.017 | 1.00 | 0.14 |
| LEU24 | H | 1.00 | 0.004 | 1.00 | -8900762.00 |
| LEU24 | HD11 | 0.88 | 0.025 | 1.00 | 0.33 |
| LEU24 | HD21 | 0.87 | 0.016 | 1.00 | 0.25 |
| LYS25 | H | 1.00 | 0.039 | 0.10 | 0.00 |

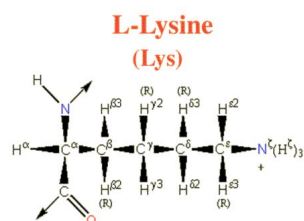


Figure 15: Image from the BMRB

Residue probability: 0.769
 Residue probability confidence: 0.942

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 174.092 | 176.660 | 3.133 | 0.000 | 0.000 |
| CA 3.25.1 | 55.646 | 57.014 | 3.028 | 0.658 | 1.000 |
| CB 3.25.2 | 34.585 | 32.981 | 3.186 | 0.936 | 1.000 |
| CG 3.25.3 | 25.106 | 24.941 | 1.956 | 0.600 | 0.909 |
| CD 3.25.4 | 29.299 | 29.020 | 2.193 | 0.811 | 0.889 |
| CE 3.25.5 | 41.649 | 41.893 | 1.492 | 0.787 | 0.875 |
| N 3.25.6 | 123.734 | 120.954 | 4.210 | 0.866 | 1.000 |
| NZ | NA | – | – | 0.000 | 0.000 |
| HA 3.25.7 | 4.847 | 4.262 | 0.489 | 0.664 | 1.000 |
| HB2 3.25.8 | 1.523 | 1.774 | 0.365 | 0.620 | 1.000 |
| HB3 3.25.9 | 1.637 | 1.742 | 0.385 | 0.502 | 1.000 |
| HG2 3.25.10 | 1.259 | 1.358 | 0.344 | 1.000 | 0.909 |
| HG3 3.25.11 | 1.199 | 1.343 | 0.357 | 0.510 | 0.909 |
| HD 3.25.12 | 1.563 | 1.614 | 0.957 | 0.643 | 0.889 |
| HE2 3.25.13 | 2.871 | 2.907 | 0.230 | 1.000 | 0.875 |
| HE3 3.25.14 | 2.762 | 2.901 | 0.241 | 1.000 | 0.875 |
| H 3.25.15 | 8.058 | 8.185 | 0.605 | 0.933 | 1.000 |
| HZ | NA | – | – | 0.000 | 0.000 |

3.25.1 Detailed Probabilities of LYS25CA:

Overall probability: 0.658
 Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU24 | 0.00 | 1.00 |
| LYS25 | 0.77 | 1.00 |
| PHE26 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L24HA | 1.00 |
| K25HB2 | 1.00 |
| K25HB3 | 1.00 |
| K25HG2 | 1.00 |
| K25HG3 | 1.00 |
| K25HD2 | 0.98 |
| K25H | 1.00 |
| K25HA | 1.00 |
| F26HA | 1.00 |
| F26H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU24 | HA | 1.00 | 0.400 | 0.00 | 0.00 |
| LYS25 | HA | 1.00 | 0.015 | 1.00 | 1.16 |
| LYS25 | HB2 | 1.00 | 0.071 | 0.00 | 0.00 |
| LYS25 | HB3 | 1.00 | 0.024 | 1.00 | 1.06 |
| LYS25 | HG2 | 1.00 | 0.006 | 1.00 | 0.38 |
| LYS25 | HG3 | 1.00 | 0.029 | 1.00 | 0.61 |
| LYS25 | HD2 | 0.98 | 0.031 | 0.90 | 0.00 |
| LYS25 | H | 1.00 | 0.063 | 0.00 | 0.00 |
| LYS25 | HE2 | 0.77 | 0.010 | 1.00 | 0.23 |
| LYS25 | HE3 | 0.76 | 0.008 | 1.00 | 0.11 |
| PHE26 | HA | 1.00 | 0.027 | 1.00 | 1.16 |
| PHE26 | H | 1.00 | 0.049 | 0.00 | 0.00 |

3.25.2 Detailed Probabilities of LYS25CB:

Overall probability: 0.936

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS25 | 0.92 | 1.00 |
| PHE26 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K25HA | 1.00 |
| K25HB2 | 1.00 |
| K25HG2 | 1.00 |
| K25HG3 | 1.00 |
| K25HD2 | 1.00 |
| K25HE2 | 0.99 |
| K25HE3 | 0.99 |
| K25H | 1.00 |
| K25HB3 | 1.00 |
| F26H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS25 | HA | 1.00 | 0.009 | 1.00 | 0.27 |
| LYS25 | HB2 | 1.00 | 0.006 | 1.00 | 2.42 |
| LYS25 | HB3 | 1.00 | 0.001 | 1.00 | 3.07 |
| LYS25 | HG2 | 1.00 | 0.027 | 1.00 | 0.46 |
| LYS25 | HG3 | 1.00 | 0.033 | 0.70 | 0.00 |
| LYS25 | HD2 | 1.00 | 0.034 | 0.60 | 0.00 |
| LYS25 | HE2 | 0.99 | 0.002 | 1.00 | 0.10 |
| LYS25 | HE3 | 0.99 | 0.006 | 1.00 | 0.07 |
| LYS25 | H | 1.00 | 0.010 | 1.00 | 0.41 |
| PHE26 | H | 1.00 | 0.009 | 1.00 | 0.10 |
| PHE26 | HA | 0.87 | 0.003 | 1.00 | 0.27 |

3.25.3 Detailed Probabilities of LYS25CG:

Overall probability: 0.600

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS25 | 0.56 | 0.90 |
| PHE26 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K25HA | 1.00 |
| K25HB2 | 1.00 |
| K25HB3 | 1.00 |
| K25HG2 | 1.00 |
| K25HD2 | 1.00 |
| K25HE2 | 1.00 |
| K25HE3 | 1.00 |
| K25H | 1.00 |
| K25HZ2 | 1.00 |
| K25HG3 | 1.00 |
| F26H | 0.96 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS25 | HA | 1.00 | 0.014 | 1.00 | 0.22 |
| LYS25 | HB2 | 1.00 | 0.283 | 0.00 | 0.00 |
| LYS25 | HB3 | 1.00 | 0.349 | 0.00 | 0.00 |
| LYS25 | HG2 | 1.00 | 0.019 | 1.00 | 3.52 |
| LYS25 | HG3 | 1.00 | 0.041 | 0.00 | 0.00 |
| LYS25 | HD2 | 1.00 | 0.323 | 0.00 | 0.00 |
| LYS25 | HE2 | 1.00 | 0.004 | 1.00 | 0.16 |
| LYS25 | HE3 | 1.00 | 0.016 | 1.00 | 0.16 |
| LYS25 | H | 1.00 | 0.009 | 1.00 | 0.07 |
| PHE26 | H | 0.96 | 0.004 | 1.00 | 0.09 |

3.25.4 Detailed Probabilities of LYS25CD:

Overall probability: 0.811

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS25 | 0.81 | 0.89 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K25HA | 0.98 |
| K25HB2 | 1.00 |
| K25HB3 | 1.00 |
| K25HG2 | 1.00 |
| K25HG3 | 1.00 |
| K25HD3 | 1.00 |
| K25HE2 | 1.00 |
| K25HE3 | 1.00 |
| K25HZ2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS25 | HA | 0.98 | 0.037 | 0.30 | 0.00 |
| LYS25 | HB2 | 1.00 | 0.020 | 1.00 | 25.27 |
| LYS25 | HB3 | 1.00 | 0.073 | 0.00 | 0.00 |
| LYS25 | HG2 | 1.00 | 0.030 | 1.00 | 1.82 |
| LYS25 | HG3 | 1.00 | 0.030 | 1.00 | 0.00 |
| LYS25 | HD2 | 1.00 | 0.001 | 1.00 | 36.33 |
| LYS25 | HE2 | 1.00 | 0.007 | 1.00 | 1.06 |
| LYS25 | HE3 | 1.00 | 0.005 | 1.00 | 0.70 |
| LYS25 | H | 0.87 | 0.007 | 1.00 | 0.09 |

3.25.5 Detailed Probabilities of LYS25CE:

Overall probability: 0.787

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS25 | 0.79 | 0.88 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K25HB2 | 0.98 |
| K25HB3 | 0.99 |
| K25HG2 | 1.00 |
| K25HG3 | 1.00 |
| K25HD2 | 1.00 |
| K25HE3 | 1.00 |
| K25HZ2 | 1.00 |
| K25HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS25 | HB2 | 0.98 | 0.022 | 1.00 | 1.69 |
| LYS25 | HB3 | 0.99 | 0.092 | 0.01 | 0.00 |
| LYS25 | HG2 | 1.00 | 0.025 | 1.00 | 0.50 |
| LYS25 | HG3 | 1.00 | 0.035 | 0.50 | 0.00 |
| LYS25 | HD2 | 1.00 | 0.018 | 1.00 | 1.69 |
| LYS25 | HE2 | 1.00 | 0.021 | 1.00 | 88.59 |
| LYS25 | HE3 | 1.00 | 0.001 | 1.00 | 7.74 |

3.25.6 Detailed Probabilities of LYS25N:

Overall probability: 0.866

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU24 | 0.85 | 1.00 |
| LYS25 | 0.84 | 1.00 |
| PHE26 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L24HA | 1.00 |
| L24H | 1.00 |
| L24HB3 | 1.00 |
| L24HB2 | 1.00 |
| L24HG | 0.98 |
| K25HA | 1.00 |
| K25HB2 | 1.00 |
| K25HB3 | 1.00 |
| K25HG2 | 1.00 |
| K25HG3 | 1.00 |
| K25H | 1.00 |
| F26H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU24 | HA | 1.00 | 0.000 | 1.00 | -1954649.00 |
| LEU24 | HB2 | 1.00 | 0.006 | 1.00 | -632202.00 |
| LEU24 | HB3 | 1.00 | 0.002 | 1.00 | -179511.00 |
| LEU24 | HG | 0.98 | 0.000 | 1.00 | -632202.00 |
| LEU24 | H | 1.00 | 0.039 | 0.10 | 0.00 |
| LEU24 | HD11 | 0.52 | 0.000 | 1.00 | -702269.00 |
| LYS25 | HA | 1.00 | 0.013 | 1.00 | -382156.00 |
| LYS25 | HB2 | 1.00 | 0.005 | 1.00 | -710619.00 |
| LYS25 | HB3 | 1.00 | 0.004 | 1.00 | -825126.00 |
| LYS25 | HG2 | 1.00 | 0.011 | 1.00 | -237215.00 |
| LYS25 | HG3 | 1.00 | 0.049 | 0.00 | 0.00 |
| LYS25 | H | 1.00 | 0.010 | 1.00 | -6110496.00 |
| LYS25 | HD2 | 0.88 | 0.035 | 0.88 | 0.00 |
| PHE26 | H | 1.00 | 0.012 | 1.00 | -84489.00 |
| PHE26 | HA | 0.92 | 0.001 | 1.00 | -382156.00 |

3.25.7 Detailed Probabilities of LYS25HA:

Overall probability: 0.664

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU24 | 0.50 | 1.00 |
| LYS25 | 0.76 | 1.00 |
| PHE26 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L24HA | 1.00 |
| K25HB2 | 1.00 |
| K25HB3 | 1.00 |
| K25HG2 | 1.00 |
| K25HG3 | 1.00 |
| K25HD2 | 0.98 |
| K25H | 1.00 |
| K25HA | 1.00 |
| F26HA | 1.00 |
| F26H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU24 | HA | 1.00 | 0.104 | 0.00 | 0.00 |
| LEU24 | H | 0.89 | 0.007 | 1.00 | -111239.00 |
| LYS25 | HA | 1.00 | 0.015 | 1.00 | 1.16 |
| LYS25 | HB2 | 1.00 | 0.009 | 1.00 | 0.40 |
| LYS25 | HB3 | 1.00 | 0.009 | 1.00 | 0.27 |
| LYS25 | HG2 | 1.00 | 0.957 | 0.00 | 0.00 |
| LYS25 | HG3 | 1.00 | 0.014 | 1.00 | 0.22 |
| LYS25 | HD2 | 0.98 | 0.037 | 0.30 | 0.00 |
| LYS25 | H | 1.00 | 0.013 | 1.00 | -382156.00 |
| PHE26 | HA | 1.00 | 0.045 | 0.00 | 0.00 |
| PHE26 | H | 1.00 | 0.011 | 1.00 | -2530640.00 |

3.25.8 Detailed Probabilities of LYS25HB2:

Overall probability: 0.620

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS25 | 0.58 | 1.00 |
| PHE26 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K25HA | 1.00 |
| K25HB3 | 1.00 |
| K25HG2 | 1.00 |
| K25HG3 | 1.00 |
| K25HD2 | 1.00 |
| K25HE2 | 0.98 |
| K25HE3 | 0.99 |
| K25H | 1.00 |
| K25HB2 | 1.00 |
| F26H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS25 | HA | 1.00 | 0.071 | 0.00 | 0.00 |
| LYS25 | HB2 | 1.00 | 0.004 | 1.00 | 4.27 |
| LYS25 | HB3 | 1.00 | 0.006 | 1.00 | 2.42 |
| LYS25 | HG2 | 1.00 | 0.291 | 0.00 | 0.00 |
| LYS25 | HG3 | 1.00 | 0.283 | 0.00 | 0.00 |
| LYS25 | HD2 | 1.00 | 0.020 | 1.00 | 25.27 |
| LYS25 | HE2 | 0.98 | 0.022 | 1.00 | 1.69 |
| LYS25 | HE3 | 0.99 | 0.038 | 0.20 | 0.00 |
| LYS25 | H | 1.00 | 0.005 | 1.00 | -710619.00 |
| PHE26 | H | 1.00 | 0.014 | 1.00 | -349291.00 |

3.25.9 Detailed Probabilities of LYS25HB3:

Overall probability: 0.502

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS25 | 0.45 | 1.00 |
| PHE26 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K25HA | 1.00 |
| K25HB2 | 1.00 |
| K25HG2 | 1.00 |
| K25HG3 | 1.00 |
| K25HD2 | 1.00 |
| K25HE2 | 0.99 |
| K25HE3 | 0.99 |
| K25H | 1.00 |
| K25HB3 | 1.00 |
| F26H | 1.00 |

NOESY contacts detailed probability

3.25 LYS(25)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS25 | HA | 1.00 | 0.024 | 1.00 | 1.06 |
| LYS25 | HB2 | 1.00 | 0.005 | 1.00 | 2.32 |
| LYS25 | HB3 | 1.00 | 0.001 | 1.00 | 3.07 |
| LYS25 | HG2 | 1.00 | 0.405 | 0.00 | 0.00 |
| LYS25 | HG3 | 1.00 | 0.349 | 0.00 | 0.00 |
| LYS25 | HD2 | 1.00 | 0.073 | 0.00 | 0.00 |
| LYS25 | HE2 | 0.99 | 0.092 | 0.01 | 0.00 |
| LYS25 | HE3 | 0.99 | 0.066 | 0.01 | 0.00 |
| LYS25 | H | 1.00 | 0.004 | 1.00 | -825126.00 |
| PHE26 | H | 1.00 | 0.012 | 1.00 | -246729.00 |

3.25.10 Detailed Probabilities of LYS25HG2:

Overall probability: 1.000

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS25 | 1.00 | 0.90 |
| PHE26 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K25HA | 1.00 |
| K25HB2 | 1.00 |
| K25HB3 | 1.00 |
| K25HG3 | 1.00 |
| K25HD2 | 1.00 |
| K25HE2 | 1.00 |
| K25HE3 | 1.00 |
| K25H | 1.00 |
| K25HZ2 | 1.00 |
| K25HG2 | 1.00 |
| F26H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS25 | HA | 1.00 | 0.006 | 1.00 | 0.38 |
| LYS25 | HB2 | 1.00 | 0.020 | 1.00 | 0.50 |
| LYS25 | HB3 | 1.00 | 0.027 | 1.00 | 0.46 |
| LYS25 | HG2 | 1.00 | 0.027 | 1.00 | 3.17 |
| LYS25 | HG3 | 1.00 | 0.019 | 1.00 | 3.52 |
| LYS25 | HD2 | 1.00 | 0.030 | 1.00 | 1.82 |
| LYS25 | HE2 | 1.00 | 0.025 | 1.00 | 0.50 |
| LYS25 | HE3 | 1.00 | 0.023 | 1.00 | 0.58 |
| LYS25 | H | 1.00 | 0.011 | 1.00 | -237215.00 |
| PHE26 | H | 0.98 | 0.029 | 1.00 | -372844.00 |

3.25.11 Detailed Probabilities of LYS25HG3:

Overall probability: 0.510

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS25 | 0.47 | 0.90 |
| PHE26 | 0.90 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K25HA | 1.00 |
| K25HB2 | 1.00 |
| K25HB3 | 1.00 |
| K25HG2 | 1.00 |
| K25HD2 | 1.00 |
| K25HE2 | 1.00 |
| K25HE3 | 1.00 |
| K25H | 1.00 |
| K25HZ2 | 1.00 |
| K25HG3 | 1.00 |
| F26H | 0.96 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS25 | HA | 1.00 | 0.029 | 1.00 | 0.61 |
| LYS25 | HB2 | 1.00 | 0.040 | 0.00 | 0.00 |
| LYS25 | HB3 | 1.00 | 0.033 | 0.70 | 0.00 |
| LYS25 | HG2 | 1.00 | 0.033 | 0.70 | 0.00 |
| LYS25 | HG3 | 1.00 | 0.041 | 0.00 | 0.00 |
| LYS25 | HD2 | 1.00 | 0.030 | 1.00 | 0.00 |
| LYS25 | HE2 | 1.00 | 0.035 | 0.50 | 0.00 |
| LYS25 | HE3 | 1.00 | 0.037 | 0.30 | 0.00 |
| LYS25 | H | 1.00 | 0.049 | 0.00 | 0.00 |
| PHE26 | H | 0.96 | 0.031 | 0.90 | 0.00 |

3.25.12 Detailed Probabilities of LYS25HD2:

Overall probability: 0.643

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS25 | 0.64 | 0.89 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K25HA | 0.98 |
| K25HB2 | 1.00 |
| K25HB3 | 1.00 |
| K25HG2 | 1.00 |
| K25HG3 | 1.00 |
| K25HD3 | 1.00 |
| K25HE2 | 1.00 |
| K25HE3 | 1.00 |
| K25HZ2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS25 | HA | 0.98 | 0.031 | 0.90 | 0.00 |
| LYS25 | HB2 | 1.00 | 0.036 | 0.40 | 0.00 |
| LYS25 | HB3 | 1.00 | 0.034 | 0.60 | 0.00 |
| LYS25 | HG2 | 1.00 | 0.331 | 0.00 | 0.00 |
| LYS25 | HG3 | 1.00 | 0.323 | 0.00 | 0.00 |
| LYS25 | HD2 | 1.00 | 0.001 | 1.00 | 36.33 |
| LYS25 | HE2 | 1.00 | 0.018 | 1.00 | 1.69 |
| LYS25 | HE3 | 1.00 | 0.002 | 1.00 | 1.00 |
| LYS25 | H | 0.88 | 0.035 | 0.88 | 0.00 |

3.25.13 Detailed Probabilities of LYS25HE2:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS25 | 1.00 | 0.88 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K25HB2 | 0.98 |
| K25HB3 | 0.99 |
| K25HG2 | 1.00 |
| K25HG3 | 1.00 |
| K25HD2 | 1.00 |
| K25HE3 | 1.00 |
| K25HZ2 | 1.00 |
| K25HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS25 | HB2 | 0.98 | 0.002 | 1.00 | 0.14 |
| LYS25 | HB3 | 0.99 | 0.002 | 1.00 | 0.10 |
| LYS25 | HG2 | 1.00 | 0.004 | 1.00 | 0.15 |
| LYS25 | HG3 | 1.00 | 0.004 | 1.00 | 0.16 |
| LYS25 | HD2 | 1.00 | 0.007 | 1.00 | 1.06 |
| LYS25 | HE2 | 1.00 | 0.021 | 1.00 | 88.59 |
| LYS25 | HE3 | 1.00 | 0.024 | 1.00 | 8.55 |
| LYS25 | HA | 0.77 | 0.010 | 1.00 | 0.23 |

3.25.14 Detailed Probabilities of LYS25HE3:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS25 | 1.00 | 0.88 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K25HB2 | 0.99 |
| K25HB3 | 0.99 |
| K25HG2 | 1.00 |
| K25HG3 | 1.00 |
| K25HD2 | 1.00 |
| K25HE2 | 1.00 |
| K25HZ2 | 1.00 |
| K25HE3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS25 | HB2 | 0.99 | 0.010 | 1.00 | 0.10 |
| LYS25 | HB3 | 0.99 | 0.006 | 1.00 | 0.07 |
| LYS25 | HG2 | 1.00 | 0.004 | 1.00 | 0.14 |
| LYS25 | HG3 | 1.00 | 0.016 | 1.00 | 0.16 |
| LYS25 | HD2 | 1.00 | 0.005 | 1.00 | 0.70 |
| LYS25 | HE2 | 1.00 | 0.001 | 1.00 | 7.74 |
| LYS25 | HE3 | 1.00 | 0.001 | 1.00 | 25.44 |
| LYS25 | HA | 0.76 | 0.008 | 1.00 | 0.11 |

3.25.15 Detailed Probabilities of LYS25H:

Overall probability: 0.933

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU24 | 1.00 | 1.00 |
| LYS25 | 0.86 | 1.00 |
| PHE26 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L24HA | 1.00 |
| L24H | 1.00 |
| L24HB3 | 1.00 |
| L24HB2 | 1.00 |
| L24HG | 0.98 |
| K25HA | 1.00 |
| K25HB2 | 1.00 |
| K25HB3 | 1.00 |
| K25HG2 | 1.00 |
| K25HG3 | 1.00 |
| K25H | 1.00 |
| F26H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU24 | HA | 1.00 | 0.009 | 1.00 | 1.10 |
| LEU24 | HB2 | 1.00 | 0.007 | 1.00 | 0.20 |
| LEU24 | HB3 | 1.00 | 0.009 | 1.00 | 0.15 |
| LEU24 | HG | 0.98 | 0.006 | 1.00 | 0.18 |
| LEU24 | H | 1.00 | 0.011 | 1.00 | -126929.00 |
| LEU24 | HD11 | 0.52 | 0.007 | 1.00 | 0.61 |
| LEU24 | HD21 | 0.59 | 0.005 | 1.00 | 0.27 |
| LYS25 | HA | 1.00 | 0.063 | 0.00 | 0.00 |
| LYS25 | HB2 | 1.00 | 0.010 | 1.00 | 0.37 |
| LYS25 | HB3 | 1.00 | 0.010 | 1.00 | 0.41 |
| LYS25 | HG2 | 1.00 | 0.008 | 1.00 | 0.09 |
| LYS25 | HG3 | 1.00 | 0.009 | 1.00 | 0.07 |
| LYS25 | H | 1.00 | 0.010 | 1.00 | -6110496.00 |
| LYS25 | HD2 | 0.88 | 0.007 | 1.00 | 0.09 |
| PHE26 | H | 1.00 | 0.003 | 1.00 | -126048.00 |

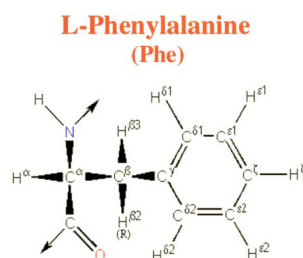
3.26 PHE(26)

Figure 16: Image from the BMRB

Residue probability: 0.895

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 175.132 | 175.508 | 2.010 | 0.000 | 0.000 |
| CA 3.26.1 | 56.569 | 58.245 | 3.808 | 0.554 | 1.000 |
| CB 3.26.2 | 40.191 | 40.078 | 3.616 | 0.889 | 1.000 |
| CD1 3.26.3 | 132.068 | 131.234 | 9.579 | 1.000 | 1.000 |
| CD2 3.26.4 | 132.294 | 131.352 | 9.581 | 1.000 | 1.000 |
| CE1 3.26.5 | 130.578 | 130.599 | 3.219 | 1.000 | 1.000 |
| CE2 3.26.6 | 130.600 | 130.633 | 2.839 | 0.715 | 1.000 |
| CZ 3.26.7 | 128.974 | 129.042 | 3.448 | 1.000 | 1.000 |
| N 3.26.8 | 123.189 | 120.315 | 4.931 | 0.871 | 1.000 |
| HA 3.26.9 | 4.835 | 4.625 | 1.237 | 0.887 | 1.000 |
| HB2 3.26.10 | 2.442 | 2.980 | 0.399 | 0.750 | 1.000 |
| HB3 3.26.11 | 3.160 | 2.916 | 0.434 | 0.889 | 1.000 |
| HD1 3.26.12 | 7.196 | 7.037 | 0.347 | 1.000 | 1.000 |
| HD2 3.26.13 | 7.196 | 7.022 | 0.417 | 1.000 | 1.000 |
| HE1 3.26.14 | 6.868 | 7.046 | 0.417 | 1.000 | 1.000 |
| HE2 3.26.15 | 6.868 | 7.043 | 0.400 | 0.857 | 1.000 |
| HZ 3.26.16 | 6.718 | 6.984 | 1.598 | 1.000 | 1.000 |
| H 3.26.17 | 9.629 | 8.375 | 0.710 | 0.803 | 1.000 |

3.26.1 Detailed Probabilities of PHE26CA:

Overall probability: 0.554

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS25 | 0.33 | 1.00 |
| PHE26 | 0.57 | 1.00 |
| ILE27 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K25HA | 1.00 |
| F26HB2 | 1.00 |
| F26HB3 | 1.00 |
| F26HD1 | 1.00 |
| F26HD2 | 1.00 |
| F26H | 1.00 |
| F26HA | 1.00 |
| I27H | 1.00 |
| I27HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS25 | HA | 1.00 | 0.045 | 0.00 | 0.00 |
| LYS25 | HB2 | 0.65 | 0.034 | 0.65 | 0.00 |
| PHE26 | HA | 1.00 | 0.057 | 0.00 | 0.00 |
| PHE26 | HB2 | 1.00 | 0.113 | 0.00 | 0.00 |
| PHE26 | HB3 | 1.00 | 0.002 | 1.00 | 0.60 |
| PHE26 | HD1 | 1.00 | 0.001 | 1.00 | 0.09 |
| PHE26 | HD2 | 1.00 | 0.001 | 1.00 | 0.09 |
| PHE26 | H | 1.00 | 0.125 | 0.00 | 0.00 |
| PHE26 | HE1 | 0.74 | 0.018 | 1.00 | 0.44 |
| ILE27 | HA | 1.00 | 0.027 | 1.00 | 0.52 |
| ILE27 | H | 1.00 | 0.106 | 0.00 | 0.00 |
| ILE27 | HB | 0.53 | 0.022 | 1.00 | 0.24 |

3.26.2 Detailed Probabilities of PHE26CB:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE26 | 1.00 | 1.00 |
| ILE27 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F26HA | 1.00 |
| F26HB2 | 1.00 |
| F26HD1 | 1.00 |
| F26HD2 | 1.00 |
| F26HE2 | 1.00 |
| F26H | 1.00 |
| F26HB3 | 1.00 |
| I27H | 1.00 |

NOESY contacts detailed probability

3.26 PHE(26)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE26 | HA | 1.00 | 0.003 | 1.00 | 0.21 |
| PHE26 | HB2 | 1.00 | 0.002 | 1.00 | 0.87 |
| PHE26 | HB3 | 1.00 | 0.008 | 1.00 | 0.88 |
| PHE26 | HD1 | 1.00 | 0.002 | 1.00 | 0.40 |
| PHE26 | HD2 | 1.00 | 0.002 | 1.00 | 0.40 |
| PHE26 | HE2 | 1.00 | 0.022 | 1.00 | 0.06 |
| PHE26 | H | 1.00 | 0.002 | 1.00 | 0.20 |
| PHE26 | HE1 | 0.89 | 0.022 | 1.00 | 0.06 |
| ILE27 | H | 1.00 | 0.095 | 0.00 | 0.00 |

3.26.3 Detailed Probabilities of PHE26CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE26 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F26HA | 1.00 |
| F26HB2 | 1.00 |
| F26HB3 | 1.00 |
| F26HD2 | 1.00 |
| F26HE1 | 1.00 |
| F26HE2 | 1.00 |
| F26HZ | 1.00 |
| F26H | 1.00 |
| F26HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE26 | HA | 1.00 | 0.001 | 1.00 | 0.59 |
| PHE26 | HB2 | 1.00 | 0.006 | 1.00 | 0.09 |
| PHE26 | HB3 | 1.00 | 0.025 | 1.00 | 1.16 |
| PHE26 | HD1 | 1.00 | 0.006 | 1.00 | 41.74 |
| PHE26 | HD2 | 1.00 | 0.006 | 1.00 | 41.74 |
| PHE26 | HE1 | 1.00 | 0.001 | 1.00 | 1.88 |
| PHE26 | HE2 | 1.00 | 0.001 | 1.00 | 1.88 |
| PHE26 | HZ | 1.00 | 0.003 | 1.00 | 0.33 |
| PHE26 | H | 1.00 | 0.004 | 1.00 | 0.11 |

3.26.4 Detailed Probabilities of PHE26CD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE26 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F26HA | 1.00 |
| F26HB2 | 1.00 |
| F26HB3 | 1.00 |
| F26HD1 | 1.00 |
| F26HE1 | 1.00 |
| F26HE2 | 1.00 |
| F26HZ | 1.00 |
| F26H | 0.99 |
| F26HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE26 | HA | 1.00 | 0.001 | 1.00 | 0.59 |
| PHE26 | HB2 | 1.00 | 0.006 | 1.00 | 0.09 |
| PHE26 | HB3 | 1.00 | 0.025 | 1.00 | 1.16 |
| PHE26 | HD1 | 1.00 | 0.006 | 1.00 | 41.74 |
| PHE26 | HD2 | 1.00 | 0.006 | 1.00 | 41.74 |
| PHE26 | HE1 | 1.00 | 0.001 | 1.00 | 1.88 |
| PHE26 | HE2 | 1.00 | 0.001 | 1.00 | 1.88 |
| PHE26 | HZ | 1.00 | 0.003 | 1.00 | 0.33 |
| PHE26 | H | 0.99 | 0.004 | 1.00 | 0.11 |

3.26.5 Detailed Probabilities of PHE26CE1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE26 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F26HD1 | 1.00 |
| F26HD2 | 1.00 |
| F26HE2 | 1.00 |
| F26HZ | 1.00 |
| F26HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE26 | HD1 | 1.00 | 0.004 | 1.00 | 0.48 |
| PHE26 | HD2 | 1.00 | 0.004 | 1.00 | 0.48 |
| PHE26 | HE1 | 1.00 | 0.004 | 1.00 | 8.24 |
| PHE26 | HE2 | 1.00 | 0.004 | 1.00 | 8.24 |
| PHE26 | HZ | 1.00 | 0.010 | 1.00 | 0.43 |
| PHE26 | HA | 0.74 | 0.006 | 1.00 | 0.16 |

3.26.6 Detailed Probabilities of PHE26CE2:

Overall probability: 0.715

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE26 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F26HB2 | 1.00 |
| F26HB3 | 1.00 |
| F26HD1 | 1.00 |
| F26HD2 | 1.00 |
| F26HE1 | 1.00 |
| F26HZ | 1.00 |
| F26HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE26 | HB2 | 1.00 | 0.128 | 0.00 | 0.00 |
| PHE26 | HB3 | 1.00 | 0.649 | 0.00 | 0.00 |
| PHE26 | HD1 | 1.00 | 0.004 | 1.00 | 0.48 |
| PHE26 | HD2 | 1.00 | 0.004 | 1.00 | 0.48 |
| PHE26 | HE1 | 1.00 | 0.004 | 1.00 | 8.24 |
| PHE26 | HE2 | 1.00 | 0.004 | 1.00 | 8.24 |
| PHE26 | HZ | 1.00 | 0.010 | 1.00 | 0.43 |

3.26.7 Detailed Probabilities of PHE26CZ:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE26 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F26HD1 | 1.00 |
| F26HD2 | 1.00 |
| F26HE1 | 1.00 |
| F26HE2 | 1.00 |
| F26HZ | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE26 | HD1 | 1.00 | 0.003 | 1.00 | 0.32 |
| PHE26 | HD2 | 1.00 | 0.003 | 1.00 | 0.32 |
| PHE26 | HE1 | 1.00 | 0.001 | 1.00 | 0.54 |
| PHE26 | HE2 | 1.00 | 0.001 | 1.00 | 0.54 |
| PHE26 | HZ | 1.00 | 0.004 | 1.00 | 1.22 |

3.26.8 Detailed Probabilities of PHE26N:

Overall probability: 0.871

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS25 | 0.99 | 1.00 |
| PHE26 | 1.00 | 1.00 |
| ILE27 | 0.35 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K25HB3 | 1.00 |
| K25HG3 | 0.96 |
| K25HB2 | 1.00 |
| K25HA | 1.00 |
| K25HG2 | 0.98 |
| K25H | 1.00 |
| F26HA | 1.00 |
| F26HB2 | 1.00 |
| F26HB3 | 1.00 |
| F26HD1 | 1.00 |
| F26HD2 | 0.99 |
| F26H | 1.00 |
| I27HA | 0.96 |
| I27H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS25 | HA | 1.00 | 0.011 | 1.00 | -2530640.00 |
| LYS25 | HB2 | 1.00 | 0.014 | 1.00 | -349291.00 |
| LYS25 | HB3 | 1.00 | 0.012 | 1.00 | -246729.00 |
| LYS25 | HG2 | 0.98 | 0.029 | 1.00 | -372844.00 |
| LYS25 | HG3 | 0.96 | 0.031 | 0.90 | 0.00 |
| LYS25 | H | 1.00 | 0.003 | 1.00 | -126048.00 |
| LYS25 | HD2 | 0.54 | 0.026 | 1.00 | -349291.00 |
| PHE26 | HA | 1.00 | 0.001 | 1.00 | -2530640.00 |
| PHE26 | HB2 | 1.00 | 0.000 | 1.00 | -456352.00 |
| PHE26 | HB3 | 1.00 | 0.006 | 1.00 | -759883.00 |
| PHE26 | HD1 | 1.00 | 0.004 | 1.00 | -929524.00 |
| PHE26 | HD2 | 0.99 | 0.004 | 1.00 | -929524.00 |
| PHE26 | H | 1.00 | 0.003 | 1.00 | -6141046.00 |
| ILE27 | HA | 0.96 | 0.142 | 0.04 | 0.00 |
| ILE27 | H | 1.00 | 0.096 | 0.00 | 0.00 |
| ILE27 | HG13 | 0.53 | 0.007 | 1.00 | -372844.00 |

3.26.9 Detailed Probabilities of PHE26HA:

Overall probability: 0.887

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS25 | 1.00 | 1.00 |
| PHE26 | 0.86 | 1.00 |
| ILE27 | 0.84 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K25HA | 1.00 |
| F26HB2 | 1.00 |
| F26HB3 | 1.00 |
| F26HD1 | 1.00 |
| F26HD2 | 1.00 |
| F26H | 1.00 |
| F26HA | 1.00 |
| I27H | 1.00 |
| I27HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS25 | HA | 1.00 | 0.027 | 1.00 | 1.16 |
| LYS25 | HB2 | 0.65 | 0.003 | 1.00 | 0.40 |
| LYS25 | HB3 | 0.87 | 0.003 | 1.00 | 0.27 |
| LYS25 | H | 0.92 | 0.001 | 1.00 | -382156.00 |
| PHE26 | HA | 1.00 | 0.057 | 0.00 | 0.00 |
| PHE26 | HB2 | 1.00 | 0.003 | 1.00 | 0.29 |
| PHE26 | HB3 | 1.00 | 0.003 | 1.00 | 0.21 |
| PHE26 | HD1 | 1.00 | 0.001 | 1.00 | 0.59 |
| PHE26 | HD2 | 1.00 | 0.001 | 1.00 | 0.59 |
| PHE26 | H | 1.00 | 0.001 | 1.00 | -2530640.00 |
| PHE26 | HE1 | 0.74 | 0.006 | 1.00 | 0.16 |
| ILE27 | HA | 1.00 | 0.038 | 0.20 | 0.00 |
| ILE27 | H | 1.00 | 0.005 | 1.00 | -1414886.00 |
| ILE27 | HB | 0.53 | 0.008 | 1.00 | 0.12 |
| ILE27 | HG12 | 0.53 | 0.001 | 1.00 | 0.14 |
| ILE27 | HG13 | 0.66 | 0.012 | 1.00 | 0.24 |

3.26.10 Detailed Probabilities of PHE26HB2:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE26 | 0.71 | 1.00 |
| ILE27 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F26HA | 1.00 |
| F26HB3 | 1.00 |
| F26HD1 | 1.00 |
| F26HD2 | 1.00 |
| F26HE2 | 1.00 |
| F26H | 1.00 |
| F26HB2 | 1.00 |
| I27H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE26 | HA | 1.00 | 0.113 | 0.00 | 0.00 |
| PHE26 | HB2 | 1.00 | 0.001 | 1.00 | 1.04 |
| PHE26 | HB3 | 1.00 | 0.002 | 1.00 | 0.87 |
| PHE26 | HD1 | 1.00 | 0.006 | 1.00 | 0.09 |
| PHE26 | HD2 | 1.00 | 0.006 | 1.00 | 0.09 |
| PHE26 | HE2 | 1.00 | 0.128 | 0.00 | 0.00 |
| PHE26 | H | 1.00 | 0.000 | 1.00 | -456352.00 |
| ILE27 | H | 1.00 | 0.006 | 1.00 | -158241.00 |

3.26.11 Detailed Probabilities of PHE26HB3:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE26 | 0.86 | 1.00 |
| ILE27 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F26HA | 1.00 |
| F26HB2 | 1.00 |
| F26HD1 | 1.00 |
| F26HD2 | 1.00 |
| F26HE2 | 1.00 |
| F26H | 1.00 |
| F26HB3 | 1.00 |
| I27H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE26 | HA | 1.00 | 0.002 | 1.00 | 0.60 |
| PHE26 | HB2 | 1.00 | 0.006 | 1.00 | 0.91 |
| PHE26 | HB3 | 1.00 | 0.008 | 1.00 | 0.88 |
| PHE26 | HD1 | 1.00 | 0.025 | 1.00 | 1.16 |
| PHE26 | HD2 | 1.00 | 0.025 | 1.00 | 1.16 |
| PHE26 | HE2 | 1.00 | 0.649 | 0.00 | 0.00 |
| PHE26 | H | 1.00 | 0.006 | 1.00 | -759883.00 |
| ILE27 | H | 1.00 | 0.008 | 1.00 | -96537.00 |
| ILE27 | HA | 0.83 | 0.015 | 1.00 | 0.48 |

3.26.12 Detailed Probabilities of PHE26HD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE26 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F26HA | 1.00 |
| F26HB2 | 1.00 |
| F26HB3 | 1.00 |
| F26HD2 | 1.00 |
| F26HE1 | 1.00 |
| F26HE2 | 1.00 |
| F26HZ | 1.00 |
| F26H | 1.00 |
| F26HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE26 | HA | 1.00 | 0.001 | 1.00 | 0.09 |
| PHE26 | HB2 | 1.00 | 0.004 | 1.00 | 0.43 |
| PHE26 | HB3 | 1.00 | 0.002 | 1.00 | 0.40 |
| PHE26 | HD1 | 1.00 | 0.006 | 1.00 | 41.74 |
| PHE26 | HD2 | 1.00 | 0.006 | 1.00 | 41.74 |
| PHE26 | HE1 | 1.00 | 0.004 | 1.00 | 0.48 |
| PHE26 | HE2 | 1.00 | 0.004 | 1.00 | 0.48 |
| PHE26 | HZ | 1.00 | 0.003 | 1.00 | 0.32 |
| PHE26 | H | 1.00 | 0.004 | 1.00 | -929524.00 |

3.26.13 Detailed Probabilities of PHE26HD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE26 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F26HA | 1.00 |
| F26HB2 | 1.00 |
| F26HB3 | 1.00 |
| F26HD1 | 1.00 |
| F26HE1 | 1.00 |
| F26HE2 | 1.00 |
| F26HZ | 1.00 |
| F26H | 0.99 |
| F26HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE26 | HA | 1.00 | 0.001 | 1.00 | 0.09 |
| PHE26 | HB2 | 1.00 | 0.004 | 1.00 | 0.43 |
| PHE26 | HB3 | 1.00 | 0.002 | 1.00 | 0.40 |
| PHE26 | HD1 | 1.00 | 0.006 | 1.00 | 41.74 |
| PHE26 | HD2 | 1.00 | 0.006 | 1.00 | 41.74 |
| PHE26 | HE1 | 1.00 | 0.004 | 1.00 | 0.48 |
| PHE26 | HE2 | 1.00 | 0.004 | 1.00 | 0.48 |
| PHE26 | HZ | 1.00 | 0.003 | 1.00 | 0.32 |
| PHE26 | H | 0.99 | 0.004 | 1.00 | -929524.00 |

3.26.14 Detailed Probabilities of PHE26HE1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE26 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F26HD1 | 1.00 |
| F26HD2 | 1.00 |
| F26HE2 | 1.00 |
| F26HZ | 1.00 |
| F26HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE26 | HD1 | 1.00 | 0.001 | 1.00 | 1.88 |
| PHE26 | HD2 | 1.00 | 0.001 | 1.00 | 1.88 |
| PHE26 | HE1 | 1.00 | 0.004 | 1.00 | 8.24 |
| PHE26 | HE2 | 1.00 | 0.004 | 1.00 | 8.24 |
| PHE26 | HZ | 1.00 | 0.001 | 1.00 | 0.54 |
| PHE26 | HA | 0.74 | 0.018 | 1.00 | 0.44 |
| PHE26 | HB3 | 0.89 | 0.022 | 1.00 | 0.06 |

3.26.15 Detailed Probabilities of PHE26HE2:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE26 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F26HB2 | 1.00 |
| F26HB3 | 1.00 |
| F26HD1 | 1.00 |
| F26HD2 | 1.00 |
| F26HE1 | 1.00 |
| F26HZ | 1.00 |
| F26HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE26 | HB2 | 1.00 | 0.324 | 0.00 | 0.00 |
| PHE26 | HB3 | 1.00 | 0.022 | 1.00 | 0.06 |
| PHE26 | HD1 | 1.00 | 0.001 | 1.00 | 1.88 |
| PHE26 | HD2 | 1.00 | 0.001 | 1.00 | 1.88 |
| PHE26 | HE1 | 1.00 | 0.004 | 1.00 | 8.24 |
| PHE26 | HE2 | 1.00 | 0.004 | 1.00 | 8.24 |
| PHE26 | HZ | 1.00 | 0.001 | 1.00 | 0.54 |

3.26.16 Detailed Probabilities of PHE26HZ:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE26 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F26HD1 | 1.00 |
| F26HD2 | 1.00 |
| F26HE1 | 1.00 |
| F26HE2 | 1.00 |
| F26HZ | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE26 | HD1 | 1.00 | 0.003 | 1.00 | 0.33 |
| PHE26 | HD2 | 1.00 | 0.003 | 1.00 | 0.33 |
| PHE26 | HE1 | 1.00 | 0.010 | 1.00 | 0.43 |
| PHE26 | HE2 | 1.00 | 0.010 | 1.00 | 0.43 |
| PHE26 | HZ | 1.00 | 0.004 | 1.00 | 1.22 |

3.26.17 Detailed Probabilities of PHE26H:

Overall probability: 0.803

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS25 | 0.86 | 1.00 |
| PHE26 | 0.83 | 1.00 |
| ILE27 | 0.52 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K25HB3 | 1.00 |
| K25HG3 | 0.96 |
| K25HB2 | 1.00 |
| K25HA | 1.00 |
| K25HG2 | 0.98 |
| K25H | 1.00 |
| F26HA | 1.00 |
| F26HB2 | 1.00 |
| F26HB3 | 1.00 |
| F26HD1 | 1.00 |
| F26HD2 | 0.99 |
| F26H | 1.00 |
| I27HA | 0.96 |
| I27H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS25 | HA | 1.00 | 0.049 | 0.00 | 0.00 |
| LYS25 | HB2 | 1.00 | 0.006 | 1.00 | 0.12 |
| LYS25 | HB3 | 1.00 | 0.009 | 1.00 | 0.10 |
| LYS25 | HG2 | 0.98 | 0.009 | 1.00 | 0.10 |
| LYS25 | HG3 | 0.96 | 0.004 | 1.00 | 0.09 |
| LYS25 | H | 1.00 | 0.012 | 1.00 | -84489.00 |
| LYS25 | HD2 | 0.54 | 0.006 | 1.00 | 0.05 |
| PHE26 | HA | 1.00 | 0.125 | 0.00 | 0.00 |
| PHE26 | HB2 | 1.00 | 0.002 | 1.00 | 0.17 |
| PHE26 | HB3 | 1.00 | 0.002 | 1.00 | 0.20 |
| PHE26 | HD1 | 1.00 | 0.004 | 1.00 | 0.11 |
| PHE26 | HD2 | 0.99 | 0.004 | 1.00 | 0.11 |
| PHE26 | H | 1.00 | 0.003 | 1.00 | -6141046.00 |
| ILE27 | HA | 0.96 | 0.058 | 0.04 | 0.00 |
| ILE27 | H | 1.00 | 0.001 | 1.00 | -97592.00 |

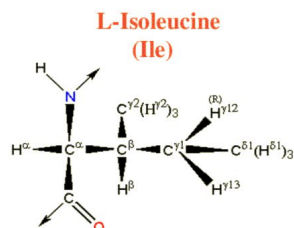


Figure 17: Image from the BMRB

Residue probability: 0.749
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|--------------|-------------|---------|--------|---------------------|--------------------|
| C | NA | – | – | 0.000 | 0.000 |
| CA 3.27.1 | 58.290 | 61.717 | 4.152 | 0.490 | 1.000 |
| CB 3.27.2 | 39.245 | 38.702 | 3.945 | 0.778 | 1.000 |
| CG1 3.27.3 | 27.157 | 27.785 | 2.037 | 0.857 | 1.000 |
| CG2 3.27.4 | 17.678 | 17.574 | 1.928 | 0.857 | 1.000 |
| CD1 3.27.5 | 13.986 | 13.545 | 3.646 | 0.857 | 1.000 |
| N 3.27.6 | 124.997 | 121.467 | 6.098 | 0.887 | 1.000 |
| HA 3.27.7 | 4.694 | 4.185 | 1.403 | 0.926 | 1.000 |
| HB 3.27.8 | 1.813 | 1.776 | 0.310 | 0.778 | 1.000 |
| HG12 3.27.9 | 0.970 | 1.271 | 0.411 | 0.471 | 1.000 |
| HG13 3.27.10 | 1.237 | 1.186 | 0.426 | 0.857 | 1.000 |
| HG2 3.27.11 | 0.918 | 0.762 | 0.283 | 0.714 | 1.000 |
| HD1 3.27.12 | 0.665 | 0.668 | 0.293 | 0.718 | 1.000 |
| H 3.27.13 | 9.301 | 8.301 | 0.685 | 0.540 | 1.000 |

3.27.1 Detailed Probabilities of ILE27CA:

Overall probability: 0.490
Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE26 | 0.41 | 1.00 |
| ILE27 | 0.58 | 1.00 |
| PRO28 | 0.37 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| F26H | 0.96 |
| F26HA | 1.00 |
| I27HB | 1.00 |
| I27HG12 | 1.00 |
| I27HG13 | 1.00 |
| I27HG21 | 1.00 |
| I27HD11 | 0.97 |
| I27H | 1.00 |
| I27HA | 1.00 |
| P28HA | 1.00 |
| P28HD2 | 1.00 |
| P28HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE26 | HA | 1.00 | 0.038 | 0.20 | 0.00 |
| PHE26 | H | 0.96 | 0.058 | 0.04 | 0.00 |
| PHE26 | HB3 | 0.83 | 0.015 | 1.00 | 0.48 |
| ILE27 | HA | 1.00 | 0.001 | 1.00 | 1.44 |
| ILE27 | HB | 1.00 | 0.002 | 1.00 | 0.44 |
| ILE27 | HG12 | 1.00 | 0.025 | 1.00 | 0.77 |
| ILE27 | HG13 | 1.00 | 0.090 | 0.00 | 0.00 |
| ILE27 | HG21 | 1.00 | 0.027 | 1.00 | 0.77 |
| ILE27 | HD11 | 0.97 | 0.280 | 0.03 | 0.00 |
| ILE27 | H | 1.00 | 0.118 | 0.00 | 0.00 |
| PRO28 | HA | 1.00 | 0.078 | 0.00 | 0.00 |
| PRO28 | HD2 | 1.00 | 0.010 | 1.00 | 1.02 |
| PRO28 | HD3 | 1.00 | 0.039 | 0.10 | 0.00 |

3.27.2 Detailed Probabilities of ILE27CB:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE27 | 0.86 | 1.00 |
| PRO28 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I27HA | 1.00 |
| I27HG12 | 1.00 |
| I27HG13 | 1.00 |
| I27HG21 | 1.00 |
| I27HD11 | 1.00 |
| I27H | 1.00 |
| I27HB | 1.00 |
| P28HD3 | 1.00 |
| P28HD2 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE27 | HA | 1.00 | 0.003 | 1.00 | 0.16 |
| ILE27 | HB | 1.00 | 0.004 | 1.00 | 3.30 |
| ILE27 | HG12 | 1.00 | 0.051 | 0.00 | 0.00 |
| ILE27 | HG13 | 1.00 | 0.008 | 1.00 | 0.40 |
| ILE27 | HG21 | 1.00 | 0.001 | 1.00 | 1.30 |
| ILE27 | HD11 | 1.00 | 0.004 | 1.00 | 0.63 |
| ILE27 | H | 1.00 | 0.007 | 1.00 | 0.39 |
| PRO28 | HD2 | 0.99 | 0.261 | 0.01 | 0.00 |
| PRO28 | HD3 | 1.00 | 0.001 | 1.00 | 0.06 |

3.27.3 Detailed Probabilities of ILE27CG1:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE27 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I27HA | 1.00 |
| I27HB | 1.00 |
| I27HG12 | 1.00 |
| I27HG21 | 1.00 |
| I27HD11 | 1.00 |
| I27H | 1.00 |
| I27HG13 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE27 | HA | 1.00 | 0.005 | 1.00 | 0.26 |
| ILE27 | HB | 1.00 | 0.024 | 1.00 | 0.61 |
| ILE27 | HG12 | 1.00 | 0.006 | 1.00 | 3.11 |
| ILE27 | HG13 | 1.00 | 0.003 | 1.00 | 10.96 |
| ILE27 | HG21 | 1.00 | 0.046 | 0.00 | 0.00 |
| ILE27 | HD11 | 1.00 | 0.002 | 1.00 | 1.12 |
| ILE27 | H | 1.00 | 0.006 | 1.00 | 0.27 |

3.27.4 Detailed Probabilities of ILE27CG2:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE27 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I27HA | 1.00 |
| I27HB | 1.00 |
| I27HG12 | 1.00 |
| I27HG13 | 1.00 |
| I27HG22 | 1.00 |
| I27HD11 | 0.99 |
| I27H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE27 | HA | 1.00 | 0.005 | 1.00 | 1.03 |
| ILE27 | HB | 1.00 | 0.010 | 1.00 | 2.37 |
| ILE27 | HG12 | 1.00 | 0.053 | 0.00 | 0.00 |
| ILE27 | HG13 | 1.00 | 0.008 | 1.00 | 0.84 |
| ILE27 | HG21 | 1.00 | 0.001 | 1.00 | 72.70 |
| ILE27 | HD11 | 0.99 | 0.001 | 1.00 | 3.70 |
| ILE27 | H | 1.00 | 0.009 | 1.00 | 0.28 |

3.27.5 Detailed Probabilities of ILE27CD1:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE27 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I27HA | 0.97 |
| I27HB | 1.00 |
| I27HG12 | 1.00 |
| I27HG13 | 1.00 |
| I27HG21 | 0.99 |
| I27HD12 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE27 | HA | 0.97 | 0.004 | 1.00 | 0.24 |
| ILE27 | HB | 1.00 | 0.006 | 1.00 | 1.10 |
| ILE27 | HG12 | 1.00 | 0.046 | 0.00 | 0.00 |
| ILE27 | HG13 | 1.00 | 0.007 | 1.00 | 1.56 |
| ILE27 | HG21 | 0.99 | 0.006 | 1.00 | 3.02 |
| ILE27 | HD11 | 1.00 | 0.006 | 1.00 | 71.18 |
| ILE27 | H | 0.94 | 0.005 | 1.00 | 0.29 |

3.27.6 Detailed Probabilities of ILE27N:

Overall probability: 0.887

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE26 | 1.00 | 1.00 |
| ILE27 | 0.90 | 1.00 |
| PRO28 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| F26HB3 | 1.00 |
| F26HA | 1.00 |
| F26HB2 | 1.00 |
| F26H | 1.00 |
| I27HA | 1.00 |
| I27HB | 1.00 |
| I27HG12 | 1.00 |
| I27HG13 | 1.00 |
| I27HG21 | 1.00 |
| I27H | 1.00 |
| P28HD2 | 0.99 |
| P28HD3 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE26 | HA | 1.00 | 0.005 | 1.00 | -1414886.00 |
| PHE26 | HB2 | 1.00 | 0.006 | 1.00 | -158241.00 |
| PHE26 | HB3 | 1.00 | 0.008 | 1.00 | -96537.00 |
| PHE26 | H | 1.00 | 0.001 | 1.00 | -97592.00 |
| PHE26 | HD1 | 0.77 | 0.001 | 1.00 | -108712.00 |
| PHE26 | HD2 | 0.64 | 0.001 | 1.00 | -108712.00 |
| ILE27 | HA | 1.00 | 0.006 | 1.00 | -233202.00 |
| ILE27 | HB | 1.00 | 0.008 | 1.00 | -631267.00 |
| ILE27 | HG12 | 1.00 | 0.037 | 0.30 | 0.00 |
| ILE27 | HG13 | 1.00 | 0.007 | 1.00 | -363176.00 |
| ILE27 | HG21 | 1.00 | 0.015 | 1.00 | -347995.00 |
| ILE27 | H | 1.00 | 0.006 | 1.00 | -3420264.00 |
| ILE27 | HD11 | 0.94 | 0.002 | 1.00 | -279991.00 |
| PRO28 | HD2 | 0.99 | 0.270 | 0.01 | 0.00 |
| PRO28 | HD3 | 0.99 | 0.008 | 1.00 | -110305.00 |

3.27.7 Detailed Probabilities of ILE27HA:

Overall probability: 0.926

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE26 | 0.52 | 1.00 |
| ILE27 | 1.00 | 1.00 |
| PRO28 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| F26H | 0.96 |
| F26HA | 1.00 |
| I27HB | 1.00 |
| I27HG12 | 1.00 |
| I27HG13 | 1.00 |
| I27HG21 | 1.00 |
| I27HD11 | 0.97 |
| I27H | 1.00 |
| I27HA | 1.00 |
| P28HA | 1.00 |
| P28HD2 | 1.00 |
| P28HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE26 | HA | 1.00 | 0.027 | 1.00 | 0.52 |
| PHE26 | H | 0.96 | 0.142 | 0.04 | 0.00 |
| ILE27 | HA | 1.00 | 0.001 | 1.00 | 1.44 |
| ILE27 | HB | 1.00 | 0.003 | 1.00 | 0.16 |
| ILE27 | HG12 | 1.00 | 0.002 | 1.00 | 0.27 |
| ILE27 | HG13 | 1.00 | 0.005 | 1.00 | 0.26 |
| ILE27 | HG21 | 1.00 | 0.005 | 1.00 | 1.03 |
| ILE27 | HD11 | 0.97 | 0.004 | 1.00 | 0.24 |
| ILE27 | H | 1.00 | 0.006 | 1.00 | -233202.00 |
| PRO28 | HA | 1.00 | 0.019 | 1.00 | 0.21 |
| PRO28 | HD2 | 1.00 | 0.005 | 1.00 | 0.63 |
| PRO28 | HD3 | 1.00 | 0.002 | 1.00 | 0.58 |
| PRO28 | HG3 | 0.88 | 0.001 | 1.00 | 0.17 |

3.27.8 Detailed Probabilities of ILE27HB:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE27 | 1.00 | 1.00 |
| PRO28 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I27HA | 1.00 |
| I27HG12 | 1.00 |
| I27HG13 | 1.00 |
| I27HG21 | 1.00 |
| I27HD11 | 1.00 |
| I27H | 1.00 |
| I27HB | 1.00 |
| P28HD3 | 1.00 |
| P28HD2 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE27 | HA | 1.00 | 0.002 | 1.00 | 0.44 |
| ILE27 | HB | 1.00 | 0.004 | 1.00 | 3.30 |
| ILE27 | HG12 | 1.00 | 0.006 | 1.00 | 0.35 |
| ILE27 | HG13 | 1.00 | 0.024 | 1.00 | 0.61 |
| ILE27 | HG21 | 1.00 | 0.010 | 1.00 | 2.37 |
| ILE27 | HD11 | 1.00 | 0.006 | 1.00 | 1.10 |
| ILE27 | H | 1.00 | 0.008 | 1.00 | -631267.00 |
| PRO28 | HD2 | 0.99 | 0.063 | 0.01 | 0.00 |
| PRO28 | HD3 | 1.00 | 0.045 | 0.00 | 0.00 |

3.27.9 Detailed Probabilities of ILE27HG12:

Overall probability: 0.471

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE27 | 0.47 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I27HA | 1.00 |
| I27HB | 1.00 |
| I27HG13 | 1.00 |
| I27HG21 | 1.00 |
| I27HD11 | 1.00 |
| I27H | 1.00 |
| I27HG12 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE27 | HA | 1.00 | 0.025 | 1.00 | 0.77 |
| ILE27 | HB | 1.00 | 0.051 | 0.00 | 0.00 |
| ILE27 | HG12 | 1.00 | 0.010 | 1.00 | 5.90 |
| ILE27 | HG13 | 1.00 | 0.006 | 1.00 | 3.11 |
| ILE27 | HG21 | 1.00 | 0.053 | 0.00 | 0.00 |
| ILE27 | HD11 | 1.00 | 0.046 | 0.00 | 0.00 |
| ILE27 | H | 1.00 | 0.037 | 0.30 | 0.00 |

3.27.10 Detailed Probabilities of ILE27HG13:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE27 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I27HA | 1.00 |
| I27HB | 1.00 |
| I27HG12 | 1.00 |
| I27HG21 | 1.00 |
| I27HD11 | 1.00 |
| I27H | 1.00 |
| I27HG13 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE27 | HA | 1.00 | 0.090 | 0.00 | 0.00 |
| ILE27 | HB | 1.00 | 0.008 | 1.00 | 0.40 |
| ILE27 | HG12 | 1.00 | 0.009 | 1.00 | 3.04 |
| ILE27 | HG13 | 1.00 | 0.003 | 1.00 | 10.96 |
| ILE27 | HG21 | 1.00 | 0.008 | 1.00 | 0.84 |
| ILE27 | HD11 | 1.00 | 0.007 | 1.00 | 1.56 |
| ILE27 | H | 1.00 | 0.007 | 1.00 | -363176.00 |

3.27.11 Detailed Probabilities of ILE27HG21:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE27 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I27HA | 1.00 |
| I27HB | 1.00 |
| I27HG12 | 1.00 |
| I27HG13 | 1.00 |
| I27HG22 | 1.00 |
| I27HD11 | 0.99 |
| I27H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE27 | HA | 1.00 | 0.027 | 1.00 | 0.77 |
| ILE27 | HB | 1.00 | 0.001 | 1.00 | 1.30 |
| ILE27 | HG12 | 1.00 | 0.042 | 0.00 | 0.00 |
| ILE27 | HG13 | 1.00 | 0.046 | 0.00 | 0.00 |
| ILE27 | HG21 | 1.00 | 0.001 | 1.00 | 72.70 |
| ILE27 | HD11 | 0.99 | 0.006 | 1.00 | 3.02 |
| ILE27 | H | 1.00 | 0.015 | 1.00 | -347995.00 |

3.27.12 Detailed Probabilities of ILE27HD11:

Overall probability: 0.718

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE27 | 0.72 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I27HA | 0.97 |
| I27HB | 1.00 |
| I27HG12 | 1.00 |
| I27HG13 | 1.00 |
| I27HG21 | 0.99 |
| I27HD12 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE27 | HA | 0.97 | 0.280 | 0.03 | 0.00 |
| ILE27 | HB | 1.00 | 0.004 | 1.00 | 0.63 |
| ILE27 | HG12 | 1.00 | 0.123 | 0.00 | 0.00 |
| ILE27 | HG13 | 1.00 | 0.002 | 1.00 | 1.12 |
| ILE27 | HG21 | 0.99 | 0.001 | 1.00 | 3.70 |
| ILE27 | HD11 | 1.00 | 0.006 | 1.00 | 71.18 |
| ILE27 | H | 0.94 | 0.002 | 1.00 | -279991.00 |

3.27.13 Detailed Probabilities of ILE27H:

Overall probability: 0.540

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE26 | 0.25 | 1.00 |
| ILE27 | 0.86 | 1.00 |
| PRO28 | 0.01 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| F26HB3 | 1.00 |
| F26HA | 1.00 |
| F26HB2 | 1.00 |
| F26H | 1.00 |
| I27HA | 1.00 |
| I27HB | 1.00 |
| I27HG12 | 1.00 |
| I27HG13 | 1.00 |
| I27HG21 | 1.00 |
| I27H | 1.00 |
| P28HD2 | 0.99 |
| P28HD3 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE26 | HA | 1.00 | 0.106 | 0.00 | 0.00 |
| PHE26 | HB2 | 1.00 | 0.002 | 1.00 | 0.06 |
| PHE26 | HB3 | 1.00 | 0.095 | 0.00 | 0.00 |
| PHE26 | H | 1.00 | 0.096 | 0.00 | 0.00 |
| ILE27 | HA | 1.00 | 0.118 | 0.00 | 0.00 |
| ILE27 | HB | 1.00 | 0.007 | 1.00 | 0.39 |
| ILE27 | HG12 | 1.00 | 0.003 | 1.00 | 0.21 |
| ILE27 | HG13 | 1.00 | 0.006 | 1.00 | 0.27 |
| ILE27 | HG21 | 1.00 | 0.009 | 1.00 | 0.28 |
| ILE27 | H | 1.00 | 0.006 | 1.00 | -3420264.00 |
| ILE27 | HD11 | 0.94 | 0.005 | 1.00 | 0.29 |
| PRO28 | HD2 | 0.99 | 0.103 | 0.01 | 0.00 |
| PRO28 | HD3 | 0.99 | 0.103 | 0.01 | 0.00 |

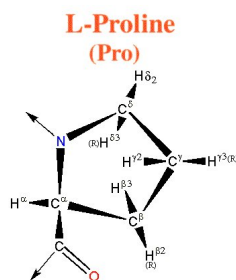
3.28 PRO(28)

Figure 18: Image from the BMRB

Residue probability: 0.725

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 174.508 | 175.173 | 13.901 | 0.000 | 0.000 |
| CA 3.28.1 | 63.045 | 62.931 | 15.301 | 0.818 | 1.000 |
| CB 3.28.2 | 32.443 | 33.632 | 13.629 | 0.669 | 1.000 |
| CG 3.28.3 | 26.610 | 28.412 | 13.801 | 0.714 | 1.000 |
| CD 3.28.4 | 50.627 | 49.797 | 3.175 | 0.819 | 1.000 |
| N | NA | - | - | 0.000 | 0.000 |
| HA 3.28.5 | 4.524 | 4.332 | 0.427 | 0.545 | 1.000 |
| HB2 3.28.6 | 1.751 | 2.099 | 0.501 | 0.605 | 1.000 |
| HB3 3.28.7 | 1.640 | 2.052 | 0.596 | 0.625 | 1.000 |
| HG2 3.28.8 | 1.944 | 1.927 | 0.364 | 0.714 | 1.000 |
| HG3 3.28.9 | 1.499 | 1.907 | 0.417 | 0.729 | 1.000 |
| HD2 3.28.10 | 3.872 | 3.640 | 0.682 | 0.847 | 1.000 |
| HD3 3.28.11 | 4.134 | 3.558 | 0.522 | 0.883 | 1.000 |

3.28.1 Detailed Probabilities of PRO28CA:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE27 | 1.00 | 1.00 |
| PRO28 | 0.71 | 1.00 |
| GLY29 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| I27HA | 1.00 |
| P28HB2 | 1.00 |
| P28HB3 | 1.00 |
| P28HG2 | 1.00 |
| P28HG3 | 1.00 |
| P28HD2 | 1.00 |
| P28HD3 | 1.00 |
| P28HA | 1.00 |
| G29HA3 | 1.00 |
| G29H | 1.00 |
| G29HA2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE27 | HA | 1.00 | 0.019 | 1.00 | 0.21 |
| PRO28 | HA | 1.00 | 0.174 | 0.00 | 0.00 |
| PRO28 | HB2 | 1.00 | 0.002 | 1.00 | 0.48 |
| PRO28 | HB3 | 1.00 | 0.002 | 1.00 | 0.33 |
| PRO28 | HG2 | 1.00 | 0.000 | 1.00 | 0.16 |
| PRO28 | HG3 | 1.00 | 0.119 | 0.00 | 0.00 |
| PRO28 | HD2 | 1.00 | 0.018 | 1.00 | 0.12 |
| PRO28 | HD3 | 1.00 | 0.018 | 1.00 | 0.42 |
| GLY29 | HA2 | 1.00 | 0.016 | 1.00 | 0.21 |
| GLY29 | HA3 | 1.00 | 0.007 | 1.00 | 0.18 |
| GLY29 | H | 1.00 | 0.012 | 1.00 | 0.26 |

3.28.2 Detailed Probabilities of PRO28CB:

Overall probability: 0.669

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO28 | 0.80 | 1.00 |
| GLY29 | 0.36 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P28HA | 1.00 |
| P28HB3 | 1.00 |
| P28HG2 | 1.00 |
| P28HG3 | 1.00 |
| P28HD2 | 1.00 |
| P28HD3 | 1.00 |
| P28HB2 | 1.00 |
| G29HA3 | 0.95 |
| G29H | 1.00 |
| G29HA2 | 0.95 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO28 | HA | 1.00 | 0.001 | 1.00 | 0.40 |
| PRO28 | HB2 | 1.00 | 0.003 | 1.00 | 10.87 |
| PRO28 | HB3 | 1.00 | 0.002 | 1.00 | 2.66 |
| PRO28 | HG2 | 1.00 | 0.024 | 1.00 | 0.45 |
| PRO28 | HG3 | 1.00 | 0.039 | 0.10 | 0.00 |
| PRO28 | HD2 | 1.00 | 0.000 | 1.00 | 0.11 |
| PRO28 | HD3 | 1.00 | 0.035 | 0.50 | 0.00 |
| GLY29 | HA2 | 0.95 | 0.230 | 0.05 | 0.00 |
| GLY29 | HA3 | 0.95 | 0.143 | 0.05 | 0.00 |
| GLY29 | H | 1.00 | 0.008 | 1.00 | 0.07 |

3.28.3 Detailed Probabilities of PRO28CG:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO28 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P28HA | 1.00 |
| P28HB2 | 1.00 |
| P28HB3 | 1.00 |
| P28HG2 | 1.00 |
| P28HD2 | 1.00 |
| P28HD3 | 1.00 |
| P28HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO28 | HA | 1.00 | 0.003 | 1.00 | 0.17 |
| PRO28 | HB2 | 1.00 | 0.189 | 0.00 | 0.00 |
| PRO28 | HB3 | 1.00 | 0.131 | 0.00 | 0.00 |
| PRO28 | HG2 | 1.00 | 0.004 | 1.00 | 2.57 |
| PRO28 | HG3 | 1.00 | 0.010 | 1.00 | 14.72 |
| PRO28 | HD2 | 1.00 | 0.002 | 1.00 | 0.54 |
| PRO28 | HD3 | 1.00 | 0.007 | 1.00 | 0.47 |

3.28.4 Detailed Probabilities of PRO28CD:

Overall probability: 0.819

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE27 | 0.50 | 1.00 |
| PRO28 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| I27H | 0.99 |
| I27HB | 1.00 |
| I27HA | 1.00 |
| P28HA | 1.00 |
| P28HB2 | 1.00 |
| P28HB3 | 1.00 |
| P28HG2 | 1.00 |
| P28HG3 | 1.00 |
| P28HD2 | 1.00 |
| P28HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE27 | HA | 1.00 | 0.002 | 1.00 | 0.58 |
| ILE27 | HB | 1.00 | 0.045 | 0.00 | 0.00 |
| ILE27 | H | 0.99 | 0.103 | 0.01 | 0.00 |
| ILE27 | HG21 | 0.84 | 0.002 | 1.00 | 0.26 |
| PRO28 | HA | 1.00 | 0.001 | 1.00 | 0.06 |
| PRO28 | HB2 | 1.00 | 0.017 | 1.00 | 0.17 |
| PRO28 | HB3 | 1.00 | 0.003 | 1.00 | 0.08 |
| PRO28 | HG2 | 1.00 | 0.005 | 1.00 | 0.36 |
| PRO28 | HG3 | 1.00 | 0.002 | 1.00 | 0.33 |
| PRO28 | HD2 | 1.00 | 0.000 | 1.00 | 1.45 |
| PRO28 | HD3 | 1.00 | 0.005 | 1.00 | 1.37 |

3.28.5 Detailed Probabilities of PRO28HA:

Overall probability: 0.545

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE27 | 0.00 | 1.00 |
| PRO28 | 0.71 | 1.00 |
| GLY29 | 0.33 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| I27HA | 1.00 |
| P28HB2 | 1.00 |
| P28HB3 | 1.00 |
| P28HG2 | 1.00 |
| P28HG3 | 1.00 |
| P28HD2 | 1.00 |
| P28HD3 | 1.00 |
| P28HA | 1.00 |
| G29HA3 | 1.00 |
| G29H | 1.00 |
| G29HA2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE27 | HA | 1.00 | 0.078 | 0.00 | 0.00 |
| PRO28 | HA | 1.00 | 0.174 | 0.00 | 0.00 |
| PRO28 | HB2 | 1.00 | 0.001 | 1.00 | 0.40 |
| PRO28 | HB3 | 1.00 | 0.219 | 0.00 | 0.00 |
| PRO28 | HG2 | 1.00 | 0.004 | 1.00 | 0.08 |
| PRO28 | HG3 | 1.00 | 0.003 | 1.00 | 0.17 |
| PRO28 | HD2 | 1.00 | 0.017 | 1.00 | 0.70 |
| PRO28 | HD3 | 1.00 | 0.001 | 1.00 | 0.06 |
| GLY29 | HA2 | 1.00 | 0.497 | 0.00 | 0.00 |
| GLY29 | HA3 | 1.00 | 0.880 | 0.00 | 0.00 |
| GLY29 | H | 1.00 | 0.000 | 1.00 | -408304.00 |

3.28.6 Detailed Probabilities of PRO28HB2:

Overall probability: 0.605

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO28 | 0.57 | 1.00 |
| GLY29 | 0.68 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P28HA | 1.00 |
| P28HB3 | 1.00 |
| P28HG2 | 1.00 |
| P28HG3 | 1.00 |
| P28HD2 | 1.00 |
| P28HD3 | 1.00 |
| P28HB2 | 1.00 |
| G29HA3 | 0.95 |
| G29H | 1.00 |
| G29HA2 | 0.95 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO28 | HA | 1.00 | 0.002 | 1.00 | 0.48 |
| PRO28 | HB2 | 1.00 | 0.003 | 1.00 | 10.87 |
| PRO28 | HB3 | 1.00 | 0.002 | 1.00 | 1.99 |
| PRO28 | HG2 | 1.00 | 0.254 | 0.00 | 0.00 |
| PRO28 | HG3 | 1.00 | 0.189 | 0.00 | 0.00 |
| PRO28 | HD2 | 1.00 | 0.124 | 0.00 | 0.00 |
| PRO28 | HD3 | 1.00 | 0.017 | 1.00 | 0.17 |
| GLY29 | HA2 | 0.95 | 0.838 | 0.05 | 0.00 |
| GLY29 | HA3 | 0.95 | 0.016 | 1.00 | 0.06 |
| GLY29 | H | 1.00 | 0.018 | 1.00 | -99919.00 |

3.28.7 Detailed Probabilities of PRO28HB3:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO28 | 0.57 | 1.00 |
| GLY29 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P28HA | 1.00 |
| P28HB2 | 1.00 |
| P28HG2 | 1.00 |
| P28HG3 | 1.00 |
| P28HD2 | 1.00 |
| P28HD3 | 1.00 |
| P28HB3 | 1.00 |
| G29H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO28 | HA | 1.00 | 0.002 | 1.00 | 0.33 |
| PRO28 | HB2 | 1.00 | 0.002 | 1.00 | 2.66 |
| PRO28 | HB3 | 1.00 | 0.109 | 0.00 | 0.00 |
| PRO28 | HG2 | 1.00 | 0.143 | 0.00 | 0.00 |
| PRO28 | HG3 | 1.00 | 0.131 | 0.00 | 0.00 |
| PRO28 | HD2 | 1.00 | 0.013 | 1.00 | 0.13 |
| PRO28 | HD3 | 1.00 | 0.003 | 1.00 | 0.08 |
| GLY29 | H | 1.00 | 0.001 | 1.00 | -85120.00 |

3.28.8 Detailed Probabilities of PRO28HG2:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO28 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P28HA | 1.00 |
| P28HB2 | 1.00 |
| P28HB3 | 1.00 |
| P28HG3 | 1.00 |
| P28HD2 | 1.00 |
| P28HD3 | 1.00 |
| P28HG2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO28 | HA | 1.00 | 0.000 | 1.00 | 0.16 |
| PRO28 | HB2 | 1.00 | 0.024 | 1.00 | 0.45 |
| PRO28 | HB3 | 1.00 | 0.156 | 0.00 | 0.00 |
| PRO28 | HG2 | 1.00 | 0.447 | 0.00 | 0.00 |
| PRO28 | HG3 | 1.00 | 0.004 | 1.00 | 2.57 |
| PRO28 | HD2 | 1.00 | 0.026 | 1.00 | 0.39 |
| PRO28 | HD3 | 1.00 | 0.005 | 1.00 | 0.36 |

3.28.9 Detailed Probabilities of PRO28HG3:

Overall probability: 0.729

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO28 | 0.73 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P28HA | 1.00 |
| P28HB2 | 1.00 |
| P28HB3 | 1.00 |
| P28HG2 | 1.00 |
| P28HD2 | 1.00 |
| P28HD3 | 1.00 |
| P28HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO28 | HA | 1.00 | 0.119 | 0.00 | 0.00 |
| PRO28 | HB2 | 1.00 | 0.039 | 0.10 | 0.00 |
| PRO28 | HB3 | 1.00 | 0.011 | 1.00 | 0.42 |
| PRO28 | HG2 | 1.00 | 0.002 | 1.00 | 2.32 |
| PRO28 | HG3 | 1.00 | 0.010 | 1.00 | 14.72 |
| PRO28 | HD2 | 1.00 | 0.002 | 1.00 | 0.38 |
| PRO28 | HD3 | 1.00 | 0.002 | 1.00 | 0.33 |

3.28.10 Detailed Probabilities of PRO28HD2:

Overall probability: 0.847

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE27 | 0.67 | 1.00 |
| PRO28 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| I27HB | 0.99 |
| I27H | 0.99 |
| I27HA | 1.00 |
| P28HA | 1.00 |
| P28HB2 | 1.00 |
| P28HB3 | 1.00 |
| P28HG2 | 1.00 |
| P28HG3 | 1.00 |
| P28HD3 | 1.00 |
| P28HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE27 | HA | 1.00 | 0.010 | 1.00 | 1.02 |
| ILE27 | HB | 0.99 | 0.261 | 0.01 | 0.00 |
| ILE27 | H | 0.99 | 0.270 | 0.01 | 0.00 |
| ILE27 | HG12 | 0.86 | 0.021 | 1.00 | 0.39 |
| ILE27 | HG13 | 0.86 | 0.023 | 1.00 | 0.25 |
| ILE27 | HG21 | 0.95 | 0.012 | 1.00 | 0.43 |
| PRO28 | HA | 1.00 | 0.018 | 1.00 | 0.12 |
| PRO28 | HB2 | 1.00 | 0.000 | 1.00 | 0.11 |
| PRO28 | HB3 | 1.00 | 0.003 | 1.00 | 0.10 |
| PRO28 | HG2 | 1.00 | 0.000 | 1.00 | 0.35 |
| PRO28 | HG3 | 1.00 | 0.002 | 1.00 | 0.54 |
| PRO28 | HD2 | 1.00 | 0.015 | 1.00 | 3.82 |
| PRO28 | HD3 | 1.00 | 0.000 | 1.00 | 1.45 |

3.28.11 Detailed Probabilities of PRO28HD3:

Overall probability: 0.883

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE27 | 0.82 | 1.00 |
| PRO28 | 0.93 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| I27H | 0.99 |
| I27HB | 1.00 |
| I27HA | 1.00 |
| P28HA | 1.00 |
| P28HB2 | 1.00 |
| P28HB3 | 1.00 |
| P28HG2 | 1.00 |
| P28HG3 | 1.00 |
| P28HD2 | 1.00 |
| P28HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE27 | HA | 1.00 | 0.039 | 0.10 | 0.00 |
| ILE27 | HB | 1.00 | 0.001 | 1.00 | 0.06 |
| ILE27 | H | 0.99 | 0.008 | 1.00 | -110305.00 |
| ILE27 | HG13 | 0.75 | 0.017 | 1.00 | 0.09 |
| ILE27 | HG21 | 0.84 | 0.002 | 1.00 | 0.38 |
| PRO28 | HA | 1.00 | 0.018 | 1.00 | 0.42 |
| PRO28 | HB2 | 1.00 | 0.035 | 0.50 | 0.00 |
| PRO28 | HB3 | 1.00 | 0.009 | 1.00 | 0.13 |
| PRO28 | HG2 | 1.00 | 0.007 | 1.00 | 0.37 |
| PRO28 | HG3 | 1.00 | 0.007 | 1.00 | 0.47 |
| PRO28 | HD2 | 1.00 | 0.001 | 1.00 | 1.32 |
| PRO28 | HD3 | 1.00 | 0.005 | 1.00 | 1.37 |

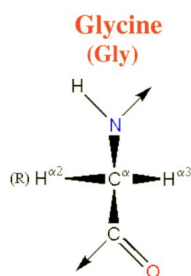
3.29 GLY(29)

Figure 19: Image from the BMRB

Residue probability: 0.785

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 172.714 | 173.872 | 2.493 | 0.000 | 0.000 |
| CA 3.29.1 | 45.432 | 45.581 | 4.381 | 0.625 | 1.000 |
| N 3.29.2 | 106.590 | 109.752 | 5.331 | 1.000 | 1.000 |
| HA2 3.29.3 | 3.642 | 3.967 | 0.380 | 0.721 | 1.000 |
| HA3 3.29.4 | 4.026 | 3.897 | 0.390 | 0.578 | 1.000 |
| H 3.29.5 | 7.989 | 8.343 | 0.939 | 1.000 | 1.000 |

3.29.1 Detailed Probabilities of GLY29CA:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO28 | 0.50 | 1.00 |
| GLY29 | 0.67 | 1.00 |
| LYS30 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P28HA | 1.00 |
| P28HB2 | 0.95 |
| G29HA2 | 1.00 |
| G29H | 1.00 |
| G29HA3 | 1.00 |
| K30HA | 1.00 |
| K30H | 1.00 |

NOESY contacts detailed probability

3.29 GLY(29)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO28 | HA | 1.00 | 0.880 | 0.00 | 0.00 |
| PRO28 | HB2 | 0.95 | 0.016 | 1.00 | 0.06 |
| GLY29 | HA2 | 1.00 | 0.002 | 1.00 | 1.45 |
| GLY29 | HA3 | 1.00 | 0.382 | 0.00 | 0.00 |
| GLY29 | H | 1.00 | 0.005 | 1.00 | 0.30 |
| LYS30 | HA | 1.00 | 1.009 | 0.00 | 0.00 |
| LYS30 | H | 1.00 | 0.005 | 1.00 | 0.13 |
| LYS30 | HB2 | 0.65 | 0.015 | 1.00 | 0.06 |

3.29.2 Detailed Probabilities of GLY29N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO28 | 1.00 | 1.00 |
| GLY29 | 1.00 | 1.00 |
| LYS30 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P28HB3 | 1.00 |
| P28HB2 | 1.00 |
| P28HA | 1.00 |
| G29HA2 | 1.00 |
| G29HA3 | 1.00 |
| G29H | 1.00 |
| K30H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO28 | HA | 1.00 | 0.000 | 1.00 | -408304.00 |
| PRO28 | HB2 | 1.00 | 0.018 | 1.00 | -99919.00 |
| PRO28 | HB3 | 1.00 | 0.001 | 1.00 | -85120.00 |
| PRO28 | HG2 | 0.88 | 0.003 | 1.00 | -87238.00 |
| PRO28 | HD2 | 0.70 | 0.004 | 1.00 | -119708.00 |
| PRO28 | HD3 | 0.62 | 0.004 | 1.00 | -269829.00 |
| GLY29 | HA2 | 1.00 | 0.001 | 1.00 | -602955.00 |
| GLY29 | HA3 | 1.00 | 0.001 | 1.00 | -510774.00 |
| GLY29 | H | 1.00 | 0.002 | 1.00 | -2259596.00 |
| LYS30 | H | 1.00 | 0.002 | 1.00 | -563926.00 |
| LYS30 | HA | 0.88 | 0.029 | 1.00 | -281946.00 |
| LYS30 | HB2 | 0.61 | 0.013 | 1.00 | -99919.00 |

3.29.3 Detailed Probabilities of GLY29HA2:

Overall probability: 0.721

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO28 | 0.52 | 1.00 |
| GLY29 | 1.00 | 1.00 |
| LYS30 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P28HB2 | 0.95 |
| P28HA | 1.00 |
| G29HA3 | 1.00 |
| G29H | 1.00 |
| G29HA2 | 1.00 |
| K30HA | 1.00 |
| K30H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO28 | HA | 1.00 | 0.016 | 1.00 | 0.21 |
| PRO28 | HB2 | 0.95 | 0.230 | 0.05 | 0.00 |
| GLY29 | HA2 | 1.00 | 0.003 | 1.00 | 2.34 |
| GLY29 | HA3 | 1.00 | 0.002 | 1.00 | 1.45 |
| GLY29 | H | 1.00 | 0.001 | 1.00 | -602955.00 |
| LYS30 | HA | 1.00 | 0.050 | 0.00 | 0.00 |
| LYS30 | H | 1.00 | 0.001 | 1.00 | -469678.00 |

3.29.4 Detailed Probabilities of GLY29HA3:

Overall probability: 0.578

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO28 | 0.52 | 1.00 |
| GLY29 | 0.67 | 1.00 |
| LYS30 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P28HA | 1.00 |
| P28HB2 | 0.95 |
| G29HA2 | 1.00 |
| G29H | 1.00 |
| G29HA3 | 1.00 |
| K30HA | 1.00 |
| K30H | 1.00 |

NOESY contacts detailed probability

3.29 GLY(29)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO28 | HA | 1.00 | 0.007 | 1.00 | 0.18 |
| PRO28 | HB2 | 0.95 | 0.143 | 0.05 | 0.00 |
| GLY29 | HA2 | 1.00 | 0.001 | 1.00 | 1.75 |
| GLY29 | HA3 | 1.00 | 0.382 | 0.00 | 0.00 |
| GLY29 | H | 1.00 | 0.001 | 1.00 | -510774.00 |
| LYS30 | HA | 1.00 | 0.051 | 0.00 | 0.00 |
| LYS30 | H | 1.00 | 0.002 | 1.00 | -344557.00 |

3.29.5 Detailed Probabilities of GLY29H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO28 | 1.00 | 1.00 |
| GLY29 | 1.00 | 1.00 |
| LYS30 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P28HB3 | 1.00 |
| P28HB2 | 1.00 |
| P28HA | 1.00 |
| G29HA2 | 1.00 |
| G29HA3 | 1.00 |
| G29H | 1.00 |
| K30H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO28 | HA | 1.00 | 0.012 | 1.00 | 0.26 |
| PRO28 | HB2 | 1.00 | 0.008 | 1.00 | 0.07 |
| PRO28 | HB3 | 1.00 | 0.004 | 1.00 | 0.09 |
| PRO28 | HG2 | 0.88 | 0.008 | 1.00 | 0.08 |
| PRO28 | HG3 | 0.68 | 0.010 | 1.00 | 0.06 |
| PRO28 | HD2 | 0.70 | 0.011 | 1.00 | 0.06 |
| PRO28 | HD3 | 0.62 | 0.007 | 1.00 | 0.08 |
| GLY29 | HA2 | 1.00 | 0.004 | 1.00 | 0.39 |
| GLY29 | HA3 | 1.00 | 0.005 | 1.00 | 0.30 |
| GLY29 | H | 1.00 | 0.002 | 1.00 | -2259596.00 |
| LYS30 | H | 1.00 | 0.002 | 1.00 | -891391.00 |

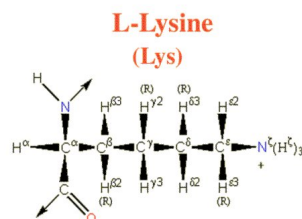
3.30 LYS(30)

Figure 20: Image from the BMRB

Residue probability: 0.920

Residue probability confidence: 0.941

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | NA | – | – | 0.000 | 0.000 |
| CA 3.30.1 | 52.700 | 57.014 | 3.028 | 0.721 | 1.000 |
| CB 3.30.2 | 34.266 | 32.981 | 3.186 | 1.000 | 1.000 |
| CG 3.30.3 | 24.103 | 24.941 | 1.956 | 1.000 | 0.900 |
| CD 3.30.4 | 28.780 | 29.020 | 2.193 | 1.000 | 0.889 |
| CE 3.30.5 | 41.780 | 41.893 | 1.492 | 0.929 | 0.875 |
| N 3.30.6 | 117.771 | 120.954 | 4.210 | 0.910 | 1.000 |
| NZ | NA | – | – | 0.000 | 0.000 |
| HA 3.30.7 | 4.653 | 4.262 | 0.489 | 0.800 | 1.000 |
| HB2 3.30.8 | 1.782 | 1.774 | 0.365 | 0.891 | 1.000 |
| HB3 3.30.9 | 1.016 | 1.742 | 0.385 | 0.792 | 1.000 |
| HG2 3.30.10 | 1.140 | 1.358 | 0.344 | 1.000 | 0.900 |
| HG3 3.30.11 | 1.139 | 1.343 | 0.357 | 1.000 | 0.900 |
| HD2 3.30.12 | 1.397 | 1.614 | 0.957 | 0.877 | 0.889 |
| HD3 3.30.13 | 1.544 | 1.595 | 0.387 | 1.000 | 0.889 |
| HE 3.30.14 | 2.854 | 2.907 | 0.230 | 0.875 | 0.875 |
| H 3.30.15 | 6.801 | 8.185 | 0.605 | 1.000 | 1.000 |
| HZ | NA | – | – | 0.000 | 0.000 |

3.30.1 Detailed Probabilities of LYS30CA:

Overall probability: 0.721

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLY29 | 0.00 | 1.00 |
| LYS30 | 0.76 | 1.00 |
| PRO31 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| G29HA2 | 1.00 |
| G29HA3 | 1.00 |
| K30HB2 | 1.00 |
| K30HB3 | 1.00 |
| K30HG2 | 1.00 |
| K30HG3 | 1.00 |
| K30HD2 | 0.98 |
| K30HD3 | 0.98 |
| K30H | 1.00 |
| K30HA | 1.00 |
| P31HD3 | 1.00 |
| P31HA | 1.00 |
| P31HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLY29 | HA2 | 1.00 | 0.050 | 0.00 | 0.00 |
| GLY29 | HA3 | 1.00 | 0.051 | 0.00 | 0.00 |
| LYS30 | HA | 1.00 | 0.008 | 1.00 | 5.99 |
| LYS30 | HB2 | 1.00 | 0.032 | 0.80 | 0.00 |
| LYS30 | HB3 | 1.00 | 0.133 | 0.00 | 0.00 |
| LYS30 | HG2 | 1.00 | 0.009 | 1.00 | 0.53 |
| LYS30 | HG3 | 1.00 | 0.010 | 1.00 | 0.53 |
| LYS30 | HD2 | 0.98 | 0.147 | 0.02 | 0.00 |
| LYS30 | HD3 | 0.98 | 0.002 | 1.00 | 0.17 |
| LYS30 | H | 1.00 | 0.018 | 1.00 | 0.23 |
| LYS30 | HE2 | 0.77 | 0.030 | 1.00 | 0.00 |
| PRO31 | HA | 1.00 | 0.006 | 1.00 | 0.12 |
| PRO31 | HD2 | 1.00 | 0.008 | 1.00 | 1.58 |
| PRO31 | HD3 | 1.00 | 0.002 | 1.00 | 0.94 |
| PRO31 | HG2 | 0.93 | 0.025 | 1.00 | 0.14 |

3.30.2 Detailed Probabilities of LYS30CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS30 | 1.00 | 1.00 |
| PRO31 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K30HA | 1.00 |
| K30HB2 | 1.00 |
| K30HG2 | 1.00 |
| K30HG3 | 1.00 |
| K30HD2 | 1.00 |
| K30HD3 | 1.00 |
| K30HE2 | 0.99 |
| K30H | 1.00 |
| K30HB3 | 1.00 |
| P31HD2 | 0.99 |
| P31HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS30 | HA | 1.00 | 0.007 | 1.00 | 0.32 |
| LYS30 | HB2 | 1.00 | 0.006 | 1.00 | 2.64 |
| LYS30 | HB3 | 1.00 | 0.005 | 1.00 | 3.01 |
| LYS30 | HG2 | 1.00 | 0.002 | 1.00 | 1.16 |
| LYS30 | HG3 | 1.00 | 0.003 | 1.00 | 1.16 |
| LYS30 | HD2 | 1.00 | 0.014 | 1.00 | 0.17 |
| LYS30 | HD3 | 1.00 | 0.010 | 1.00 | 0.20 |
| LYS30 | HE2 | 0.99 | 0.005 | 1.00 | 0.09 |
| LYS30 | H | 1.00 | 0.004 | 1.00 | 0.22 |
| PRO31 | HD2 | 0.99 | 0.006 | 1.00 | 0.20 |
| PRO31 | HD3 | 1.00 | 0.000 | 1.00 | 0.33 |

3.30.3 Detailed Probabilities of LYS30CG:

Overall probability: 1.000

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS30 | 1.00 | 0.90 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K30HA | 1.00 |
| K30HB2 | 1.00 |
| K30HB3 | 1.00 |
| K30HG3 | 1.00 |
| K30HD2 | 1.00 |
| K30HD3 | 1.00 |
| K30HE2 | 1.00 |
| K30H | 1.00 |
| K30HZ2 | 1.00 |
| K30HG2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS30 | HA | 1.00 | 0.003 | 1.00 | 0.39 |
| LYS30 | HB2 | 1.00 | 0.005 | 1.00 | 1.01 |
| LYS30 | HB3 | 1.00 | 0.009 | 1.00 | 1.29 |
| LYS30 | HG2 | 1.00 | 0.000 | 1.00 | 15.70 |
| LYS30 | HG3 | 1.00 | 0.001 | 1.00 | 15.70 |
| LYS30 | HD2 | 1.00 | 0.018 | 1.00 | 0.55 |
| LYS30 | HD3 | 1.00 | 0.008 | 1.00 | 0.45 |
| LYS30 | HE2 | 1.00 | 0.007 | 1.00 | 0.51 |
| LYS30 | H | 1.00 | 0.003 | 1.00 | 0.20 |

3.30.4 Detailed Probabilities of LYS30CD:

Overall probability: 1.000

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS30 | 1.00 | 0.89 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K30HA | 0.98 |
| K30HB2 | 1.00 |
| K30HB3 | 1.00 |
| K30HG2 | 1.00 |
| K30HG3 | 1.00 |
| K30HD3 | 1.00 |
| K30HE2 | 1.00 |
| K30HZ2 | 1.00 |
| K30HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS30 | HA | 0.98 | 0.000 | 1.00 | 0.13 |
| LYS30 | HB2 | 1.00 | 0.000 | 1.00 | 0.37 |
| LYS30 | HB3 | 1.00 | 0.007 | 1.00 | 0.24 |
| LYS30 | HG2 | 1.00 | 0.015 | 1.00 | 0.80 |
| LYS30 | HG3 | 1.00 | 0.016 | 1.00 | 0.80 |
| LYS30 | HD2 | 1.00 | 0.010 | 1.00 | 18.73 |
| LYS30 | HD3 | 1.00 | 0.006 | 1.00 | 4.14 |
| LYS30 | HE2 | 1.00 | 0.008 | 1.00 | 0.77 |
| LYS30 | H | 0.88 | 0.000 | 1.00 | 0.05 |

3.30.5 Detailed Probabilities of LYS30CE:

Overall probability: 0.929

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS30 | 0.93 | 0.88 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K30HB2 | 0.98 |
| K30HB3 | 0.99 |
| K30HG2 | 1.00 |
| K30HG3 | 1.00 |
| K30HD2 | 1.00 |
| K30HD3 | 1.00 |
| K30HE3 | 1.00 |
| K30HZ2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS30 | HB2 | 0.99 | 0.006 | 1.00 | 0.51 |
| LYS30 | HB3 | 0.99 | 0.035 | 0.50 | 0.00 |
| LYS30 | HG2 | 1.00 | 0.004 | 1.00 | 1.20 |
| LYS30 | HG3 | 1.00 | 0.005 | 1.00 | 1.20 |
| LYS30 | HD2 | 1.00 | 0.005 | 1.00 | 1.04 |
| LYS30 | HD3 | 1.00 | 0.001 | 1.00 | 1.69 |
| LYS30 | HE2 | 1.00 | 0.004 | 1.00 | 88.59 |

3.30.6 Detailed Probabilities of LYS30N:

Overall probability: 0.910

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLY29 | 1.00 | 1.00 |
| LYS30 | 1.00 | 1.00 |
| PRO31 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| G29HA3 | 1.00 |
| G29HA2 | 1.00 |
| G29H | 1.00 |
| K30HA | 1.00 |
| K30HB2 | 1.00 |
| K30HB3 | 1.00 |
| K30HG2 | 1.00 |
| K30HG3 | 1.00 |
| K30H | 1.00 |
| P31HD2 | 0.99 |
| P31HD3 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLY29 | HA2 | 1.00 | 0.001 | 1.00 | -469678.00 |
| GLY29 | HA3 | 1.00 | 0.002 | 1.00 | -344557.00 |
| GLY29 | H | 1.00 | 0.002 | 1.00 | -891391.00 |
| LYS30 | HA | 1.00 | 0.007 | 1.00 | -661160.00 |
| LYS30 | HB2 | 1.00 | 0.013 | 1.00 | -764871.00 |
| LYS30 | HB3 | 1.00 | 0.007 | 1.00 | -695400.00 |
| LYS30 | HG2 | 1.00 | 0.002 | 1.00 | -626825.00 |
| LYS30 | HG3 | 1.00 | 0.003 | 1.00 | -626825.00 |
| LYS30 | H | 1.00 | 0.004 | 1.00 | -8879725.00 |
| PRO31 | HD2 | 0.99 | 0.009 | 1.00 | -149310.00 |
| PRO31 | HD3 | 0.99 | 0.081 | 0.01 | 0.00 |

3.30.7 Detailed Probabilities of LYS30HA:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLY29 | 0.33 | 1.00 |
| LYS30 | 1.00 | 1.00 |
| PRO31 | 0.75 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| G29HA2 | 1.00 |
| G29HA3 | 1.00 |
| K30HB2 | 1.00 |
| K30HB3 | 1.00 |
| K30HG2 | 1.00 |
| K30HG3 | 1.00 |
| K30HD2 | 0.98 |
| K30HD3 | 0.98 |
| K30H | 1.00 |
| K30HA | 1.00 |
| P31HD3 | 1.00 |
| P31HA | 1.00 |
| P31HD2 | 1.00 |

NOESY contacts detailed probability

3.30 LYS(30)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLY29 | HA2 | 1.00 | 0.626 | 0.00 | 0.00 |
| GLY29 | HA3 | 1.00 | 1.009 | 0.00 | 0.00 |
| GLY29 | H | 0.88 | 0.029 | 1.00 | -281946.00 |
| LYS30 | HA | 1.00 | 0.008 | 1.00 | 5.99 |
| LYS30 | HB2 | 1.00 | 0.008 | 1.00 | 0.68 |
| LYS30 | HB3 | 1.00 | 0.007 | 1.00 | 0.32 |
| LYS30 | HG2 | 1.00 | 0.003 | 1.00 | 0.39 |
| LYS30 | HG3 | 1.00 | 0.003 | 1.00 | 0.39 |
| LYS30 | HD2 | 0.98 | 0.000 | 1.00 | 0.13 |
| LYS30 | HD3 | 0.98 | 0.006 | 1.00 | 0.26 |
| LYS30 | H | 1.00 | 0.007 | 1.00 | -661160.00 |
| PRO31 | HA | 1.00 | 0.048 | 0.00 | 0.00 |
| PRO31 | HD2 | 1.00 | 0.005 | 1.00 | 1.74 |
| PRO31 | HD3 | 1.00 | 0.006 | 1.00 | 1.34 |
| PRO31 | HG3 | 0.92 | 0.010 | 1.00 | 0.37 |

3.30.8 Detailed Probabilities of LYS30HB2:

Overall probability: 0.891

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS30 | 0.87 | 1.00 |
| PRO31 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K30HA | 1.00 |
| K30HB3 | 1.00 |
| K30HG2 | 1.00 |
| K30HG3 | 1.00 |
| K30HD2 | 1.00 |
| K30HD3 | 1.00 |
| K30HE2 | 0.98 |
| K30H | 1.00 |
| K30HB2 | 1.00 |
| P31HD2 | 0.99 |
| P31HD3 | 1.00 |

NOESY contacts detailed probability

3.30 LYS(30)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS30 | HA | 1.00 | 0.032 | 0.80 | 0.00 |
| LYS30 | HB2 | 1.00 | 0.122 | 0.00 | 0.00 |
| LYS30 | HB3 | 1.00 | 0.006 | 1.00 | 2.64 |
| LYS30 | HG2 | 1.00 | 0.005 | 1.00 | 1.01 |
| LYS30 | HG3 | 1.00 | 0.005 | 1.00 | 1.01 |
| LYS30 | HD2 | 1.00 | 0.000 | 1.00 | 0.37 |
| LYS30 | HD3 | 1.00 | 0.014 | 1.00 | 0.56 |
| LYS30 | HE2 | 0.98 | 0.006 | 1.00 | 0.51 |
| LYS30 | H | 1.00 | 0.013 | 1.00 | -764871.00 |
| PRO31 | HD2 | 0.99 | 0.006 | 1.00 | 0.72 |
| PRO31 | HD3 | 1.00 | 0.005 | 1.00 | 1.05 |

3.30.9 Detailed Probabilities of LYS30HB3:

Overall probability: 0.792

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS30 | 0.72 | 1.00 |
| PRO31 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K30HA | 1.00 |
| K30HB2 | 1.00 |
| K30HG2 | 1.00 |
| K30HG3 | 1.00 |
| K30HD2 | 1.00 |
| K30HD3 | 1.00 |
| K30HE2 | 0.99 |
| K30H | 1.00 |
| K30HB3 | 1.00 |
| P31HD2 | 0.99 |
| P31HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS30 | HA | 1.00 | 0.133 | 0.00 | 0.00 |
| LYS30 | HB2 | 1.00 | 0.004 | 1.00 | 3.24 |
| LYS30 | HB3 | 1.00 | 0.005 | 1.00 | 3.01 |
| LYS30 | HG2 | 1.00 | 0.009 | 1.00 | 1.29 |
| LYS30 | HG3 | 1.00 | 0.009 | 1.00 | 1.29 |
| LYS30 | HD2 | 1.00 | 0.007 | 1.00 | 0.24 |
| LYS30 | HD3 | 1.00 | 0.140 | 0.00 | 0.00 |
| LYS30 | HE2 | 0.99 | 0.035 | 0.50 | 0.00 |
| LYS30 | H | 1.00 | 0.007 | 1.00 | -695400.00 |
| PRO31 | HD2 | 0.99 | 0.009 | 1.00 | 0.25 |
| PRO31 | HD3 | 1.00 | 0.007 | 1.00 | 0.38 |
| PRO31 | HG2 | 0.53 | 0.003 | 1.00 | 0.07 |

3.30.10 Detailed Probabilities of LYS30HG2:

Overall probability: 1.000

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS30 | 1.00 | 0.90 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K30HA | 1.00 |
| K30HB2 | 1.00 |
| K30HB3 | 1.00 |
| K30HG3 | 1.00 |
| K30HD2 | 1.00 |
| K30HD3 | 1.00 |
| K30HE2 | 1.00 |
| K30H | 1.00 |
| K30HZ2 | 1.00 |
| K30HG2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS30 | HA | 1.00 | 0.010 | 1.00 | 0.53 |
| LYS30 | HB2 | 1.00 | 0.003 | 1.00 | 1.40 |
| LYS30 | HB3 | 1.00 | 0.003 | 1.00 | 1.16 |
| LYS30 | HG2 | 1.00 | 0.001 | 1.00 | 15.70 |
| LYS30 | HG3 | 1.00 | 0.001 | 1.00 | 15.70 |
| LYS30 | HD2 | 1.00 | 0.016 | 1.00 | 0.80 |
| LYS30 | HD3 | 1.00 | 0.017 | 1.00 | 0.88 |
| LYS30 | HE2 | 1.00 | 0.005 | 1.00 | 1.20 |
| LYS30 | H | 1.00 | 0.003 | 1.00 | -626825.00 |

3.30.11 Detailed Probabilities of LYS30HG3:

Overall probability: 1.000

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS30 | 1.00 | 0.90 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K30HA | 1.00 |
| K30HB2 | 1.00 |
| K30HB3 | 1.00 |
| K30HG2 | 1.00 |
| K30HD2 | 1.00 |
| K30HD3 | 1.00 |
| K30HE2 | 1.00 |
| K30H | 1.00 |
| K30HZ2 | 1.00 |
| K30HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS30 | HA | 1.00 | 0.010 | 1.00 | 0.53 |
| LYS30 | HB2 | 1.00 | 0.003 | 1.00 | 1.40 |
| LYS30 | HB3 | 1.00 | 0.003 | 1.00 | 1.16 |
| LYS30 | HG2 | 1.00 | 0.001 | 1.00 | 15.70 |
| LYS30 | HG3 | 1.00 | 0.001 | 1.00 | 15.70 |
| LYS30 | HD2 | 1.00 | 0.016 | 1.00 | 0.80 |
| LYS30 | HD3 | 1.00 | 0.017 | 1.00 | 0.88 |
| LYS30 | HE2 | 1.00 | 0.005 | 1.00 | 1.20 |
| LYS30 | H | 1.00 | 0.003 | 1.00 | -626825.00 |

3.30.12 Detailed Probabilities of LYS30HD2:

Overall probability: 0.877

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS30 | 0.88 | 0.89 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K30HA | 0.98 |
| K30HB2 | 1.00 |
| K30HB3 | 1.00 |
| K30HG2 | 1.00 |
| K30HG3 | 1.00 |
| K30HD3 | 1.00 |
| K30HE2 | 1.00 |
| K30HZ2 | 1.00 |
| K30HD2 | 1.00 |

NOESY contacts detailed probability

3.30 LYS(30)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS30 | HA | 0.98 | 0.147 | 0.02 | 0.00 |
| LYS30 | HB2 | 1.00 | 0.010 | 1.00 | 0.23 |
| LYS30 | HB3 | 1.00 | 0.014 | 1.00 | 0.17 |
| LYS30 | HG2 | 1.00 | 0.018 | 1.00 | 0.55 |
| LYS30 | HG3 | 1.00 | 0.018 | 1.00 | 0.55 |
| LYS30 | HD2 | 1.00 | 0.010 | 1.00 | 18.73 |
| LYS30 | HD3 | 1.00 | 0.006 | 1.00 | 4.41 |
| LYS30 | HE2 | 1.00 | 0.005 | 1.00 | 1.04 |

3.30.13 Detailed Probabilities of LYS30HD3:

Overall probability: 1.000

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS30 | 1.00 | 0.89 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K30HA | 0.98 |
| K30HB2 | 1.00 |
| K30HB3 | 1.00 |
| K30HG2 | 1.00 |
| K30HG3 | 1.00 |
| K30HD2 | 1.00 |
| K30HE2 | 1.00 |
| K30HZ2 | 1.00 |
| K30HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS30 | HA | 0.98 | 0.002 | 1.00 | 0.17 |
| LYS30 | HB2 | 1.00 | 0.005 | 1.00 | 0.33 |
| LYS30 | HB3 | 1.00 | 0.010 | 1.00 | 0.20 |
| LYS30 | HG2 | 1.00 | 0.008 | 1.00 | 0.45 |
| LYS30 | HG3 | 1.00 | 0.008 | 1.00 | 0.45 |
| LYS30 | HD2 | 1.00 | 0.006 | 1.00 | 4.14 |
| LYS30 | HD3 | 1.00 | 0.001 | 1.00 | 25.27 |
| LYS30 | HE2 | 1.00 | 0.001 | 1.00 | 1.69 |

3.30.14 Detailed Probabilities of LYS30HE2:

Overall probability: 0.875

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS30 | 0.88 | 0.88 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K30HB2 | 0.98 |
| K30HB3 | 0.99 |
| K30HG2 | 1.00 |
| K30HG3 | 1.00 |
| K30HD2 | 1.00 |
| K30HD3 | 1.00 |
| K30HE3 | 1.00 |
| K30HZ2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS30 | HB2 | 0.99 | 0.000 | 1.00 | 0.13 |
| LYS30 | HB3 | 0.99 | 0.005 | 1.00 | 0.09 |
| LYS30 | HG2 | 1.00 | 0.007 | 1.00 | 0.51 |
| LYS30 | HG3 | 1.00 | 0.007 | 1.00 | 0.51 |
| LYS30 | HD2 | 1.00 | 0.008 | 1.00 | 0.77 |
| LYS30 | HD3 | 1.00 | 0.318 | 0.00 | 0.00 |
| LYS30 | HE2 | 1.00 | 0.004 | 1.00 | 88.59 |
| LYS30 | HA | 0.76 | 0.030 | 1.00 | 0.00 |

3.30.15 Detailed Probabilities of LYS30H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLY29 | 1.00 | 1.00 |
| LYS30 | 1.00 | 1.00 |
| PRO31 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| G29HA3 | 1.00 |
| G29HA2 | 1.00 |
| G29H | 1.00 |
| K30HA | 1.00 |
| K30HB2 | 1.00 |
| K30HB3 | 1.00 |
| K30HG2 | 1.00 |
| K30HG3 | 1.00 |
| K30H | 1.00 |
| P31HD2 | 0.99 |
| P31HD3 | 0.99 |

NOESY contacts detailed probability

3.30 LYS(30)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLY29 | HA2 | 1.00 | 0.001 | 1.00 | 0.21 |
| GLY29 | HA3 | 1.00 | 0.005 | 1.00 | 0.13 |
| GLY29 | H | 1.00 | 0.002 | 1.00 | -563926.00 |
| LYS30 | HA | 1.00 | 0.018 | 1.00 | 0.23 |
| LYS30 | HB2 | 1.00 | 0.001 | 1.00 | 0.22 |
| LYS30 | HB3 | 1.00 | 0.004 | 1.00 | 0.22 |
| LYS30 | HG2 | 1.00 | 0.003 | 1.00 | 0.20 |
| LYS30 | HG3 | 1.00 | 0.003 | 1.00 | 0.20 |
| LYS30 | H | 1.00 | 0.004 | 1.00 | -8879725.00 |
| LYS30 | HD2 | 0.88 | 0.000 | 1.00 | 0.05 |
| LYS30 | HD3 | 0.87 | 0.019 | 1.00 | 0.06 |
| PRO31 | HD2 | 0.99 | 0.010 | 1.00 | 0.05 |
| PRO31 | HD3 | 0.99 | 0.024 | 1.00 | 0.10 |

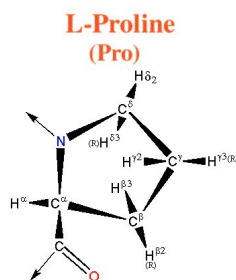


Figure 21: Image from the BMRB

Residue probability: 0.817
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 175.080 | 175.173 | 13.901 | 0.000 | 0.000 |
| CA 3.31.1 | 63.314 | 62.931 | 15.301 | 0.833 | 1.000 |
| CB 3.31.2 | 32.043 | 33.632 | 13.629 | 0.875 | 1.000 |
| CG 3.31.3 | 27.658 | 28.412 | 13.801 | 0.857 | 1.000 |
| CD 3.31.4 | 50.171 | 49.797 | 3.175 | 0.913 | 1.000 |
| N | NA | - | - | 0.000 | 0.000 |
| HA 3.31.5 | 4.336 | 4.332 | 0.427 | 0.818 | 1.000 |
| HB2 3.31.6 | 2.328 | 2.099 | 0.501 | 0.890 | 1.000 |
| HB3 3.31.7 | 1.821 | 2.052 | 0.596 | 0.663 | 1.000 |
| HG2 3.31.8 | 2.107 | 1.927 | 0.364 | 0.571 | 1.000 |
| HG3 3.31.9 | 1.972 | 1.907 | 0.417 | 0.714 | 1.000 |
| HD2 3.31.10 | 3.770 | 3.640 | 0.682 | 1.000 | 1.000 |
| HD3 3.31.11 | 3.562 | 3.558 | 0.522 | 0.847 | 1.000 |

3.31.1 Detailed Probabilities of PRO31CA:

Overall probability: 0.833
Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS30 | 0.00 | 1.00 |
| PRO31 | 1.00 | 1.00 |
| VAL32 | 0.75 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K30HA | 1.00 |
| P31HB2 | 1.00 |
| P31HB3 | 1.00 |
| P31HG2 | 1.00 |
| P31HG3 | 1.00 |
| P31HD2 | 1.00 |
| P31HD3 | 1.00 |
| P31HA | 1.00 |
| V32H | 1.00 |
| V32HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS30 | HA | 1.00 | 0.048 | 0.00 | 0.00 |
| PRO31 | HA | 1.00 | 0.001 | 1.00 | 6.90 |
| PRO31 | HB2 | 1.00 | 0.002 | 1.00 | 1.26 |
| PRO31 | HB3 | 1.00 | 0.002 | 1.00 | 0.73 |
| PRO31 | HG2 | 1.00 | 0.006 | 1.00 | 0.37 |
| PRO31 | HG3 | 1.00 | 0.002 | 1.00 | 0.40 |
| PRO31 | HD2 | 1.00 | 0.010 | 1.00 | 0.15 |
| PRO31 | HD3 | 1.00 | 0.003 | 1.00 | 0.14 |
| VAL32 | HA | 1.00 | 0.119 | 0.00 | 0.00 |
| VAL32 | H | 1.00 | 0.003 | 1.00 | 1.69 |
| VAL32 | HB | 0.51 | 0.003 | 1.00 | 0.37 |
| VAL32 | HG21 | 0.54 | 0.001 | 1.00 | 0.40 |

3.31.2 Detailed Probabilities of PRO31CB:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO31 | 0.86 | 1.00 |
| VAL32 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P31HA | 1.00 |
| P31HB2 | 1.00 |
| P31HG2 | 1.00 |
| P31HG3 | 1.00 |
| P31HD2 | 1.00 |
| P31HD3 | 1.00 |
| P31HB3 | 1.00 |
| V32H | 1.00 |

NOESY contacts detailed probability

3.31 PRO(31)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO31 | HA | 1.00 | 0.044 | 0.00 | 0.00 |
| PRO31 | HB2 | 1.00 | 0.004 | 1.00 | 3.36 |
| PRO31 | HB3 | 1.00 | 0.005 | 1.00 | 6.97 |
| PRO31 | HG2 | 1.00 | 0.007 | 1.00 | 0.97 |
| PRO31 | HG3 | 1.00 | 0.018 | 1.00 | 1.37 |
| PRO31 | HD2 | 1.00 | 0.001 | 1.00 | 0.25 |
| PRO31 | HD3 | 1.00 | 0.009 | 1.00 | 0.36 |
| VAL32 | H | 1.00 | 0.007 | 1.00 | 0.25 |

3.31.3 Detailed Probabilities of PRO31CG:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO31 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P31HA | 1.00 |
| P31HB2 | 1.00 |
| P31HB3 | 1.00 |
| P31HG2 | 1.00 |
| P31HD2 | 1.00 |
| P31HD3 | 1.00 |
| P31HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO31 | HA | 1.00 | 0.000 | 1.00 | 0.38 |
| PRO31 | HB2 | 1.00 | 0.003 | 1.00 | 0.84 |
| PRO31 | HB3 | 1.00 | 0.005 | 1.00 | 1.67 |
| PRO31 | HG2 | 1.00 | 0.002 | 1.00 | 3.30 |
| PRO31 | HG3 | 1.00 | 0.025 | 1.00 | 12.54 |
| PRO31 | HD2 | 1.00 | 0.002 | 1.00 | 0.75 |
| PRO31 | HD3 | 1.00 | 0.041 | 0.00 | 0.00 |

3.31.4 Detailed Probabilities of PRO31CD:

Overall probability: 0.913

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS30 | 1.00 | 1.00 |
| PRO31 | 0.81 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K30H | 0.99 |
| K30HB3 | 0.99 |
| K30HA | 1.00 |
| K30HB2 | 0.99 |
| P31HA | 1.00 |
| P31HB2 | 1.00 |
| P31HB3 | 1.00 |
| P31HG2 | 1.00 |
| P31HG3 | 1.00 |
| P31HD3 | 1.00 |
| P31HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS30 | HA | 1.00 | 0.005 | 1.00 | 1.74 |
| LYS30 | HB2 | 0.99 | 0.006 | 1.00 | 0.72 |
| LYS30 | HB3 | 0.99 | 0.009 | 1.00 | 0.25 |
| LYS30 | H | 0.99 | 0.010 | 1.00 | 0.05 |
| LYS30 | HG2 | 0.93 | 0.024 | 1.00 | 0.23 |
| LYS30 | HG3 | 0.92 | 0.025 | 1.00 | 0.23 |
| LYS30 | HD2 | 0.66 | 0.017 | 1.00 | 0.52 |
| LYS30 | HD3 | 0.66 | 0.001 | 1.00 | 0.09 |
| PRO31 | HA | 1.00 | 0.026 | 1.00 | 1.81 |
| PRO31 | HB2 | 1.00 | 0.000 | 1.00 | 0.36 |
| PRO31 | HB3 | 1.00 | 0.033 | 0.70 | 0.00 |
| PRO31 | HG2 | 1.00 | 0.052 | 0.00 | 0.00 |
| PRO31 | HG3 | 1.00 | 0.007 | 1.00 | 0.97 |
| PRO31 | HD2 | 1.00 | 0.002 | 1.00 | 5.09 |
| PRO31 | HD3 | 1.00 | 0.009 | 1.00 | 4.34 |

3.31.5 Detailed Probabilities of PRO31HA:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS30 | 1.00 | 1.00 |
| PRO31 | 0.86 | 1.00 |
| VAL32 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K30HA | 1.00 |
| P31HB2 | 1.00 |
| P31HB3 | 1.00 |
| P31HG2 | 1.00 |
| P31HG3 | 1.00 |
| P31HD2 | 1.00 |
| P31HD3 | 1.00 |
| P31HA | 1.00 |
| V32H | 1.00 |
| V32HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS30 | HA | 1.00 | 0.006 | 1.00 | 0.12 |
| PRO31 | HA | 1.00 | 0.001 | 1.00 | 6.90 |
| PRO31 | HB2 | 1.00 | 0.002 | 1.00 | 1.48 |
| PRO31 | HB3 | 1.00 | 0.044 | 0.00 | 0.00 |
| PRO31 | HG2 | 1.00 | 0.003 | 1.00 | 0.54 |
| PRO31 | HG3 | 1.00 | 0.000 | 1.00 | 0.38 |
| PRO31 | HD2 | 1.00 | 0.026 | 1.00 | 1.81 |
| PRO31 | HD3 | 1.00 | 0.025 | 1.00 | 1.57 |
| VAL32 | HA | 1.00 | 0.118 | 0.00 | 0.00 |
| VAL32 | H | 1.00 | 0.001 | 1.00 | -1794731.00 |
| VAL32 | HG21 | 0.54 | 0.006 | 1.00 | 0.16 |

3.31.6 Detailed Probabilities of PRO31HB2:

Overall probability: 0.890

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO31 | 1.00 | 1.00 |
| VAL32 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P31HA | 1.00 |
| P31HB3 | 1.00 |
| P31HG2 | 1.00 |
| P31HG3 | 1.00 |
| P31HD2 | 1.00 |
| P31HD3 | 1.00 |
| P31HB2 | 1.00 |
| V32HA | 0.99 |
| V32H | 1.00 |

NOESY contacts detailed probability

3.31 PRO(31)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO31 | HA | 1.00 | 0.002 | 1.00 | 1.26 |
| PRO31 | HB2 | 1.00 | 0.012 | 1.00 | 21.15 |
| PRO31 | HB3 | 1.00 | 0.004 | 1.00 | 3.36 |
| PRO31 | HG2 | 1.00 | 0.027 | 1.00 | 3.73 |
| PRO31 | HG3 | 1.00 | 0.003 | 1.00 | 0.84 |
| PRO31 | HD2 | 1.00 | 0.000 | 1.00 | 0.36 |
| PRO31 | HD3 | 1.00 | 0.002 | 1.00 | 0.35 |
| VAL32 | HA | 0.99 | 0.214 | 0.01 | 0.00 |
| VAL32 | H | 1.00 | 0.001 | 1.00 | -377089.00 |

3.31.7 Detailed Probabilities of PRO31HB3:

Overall probability: 0.663

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO31 | 0.61 | 1.00 |
| VAL32 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P31HA | 1.00 |
| P31HB2 | 1.00 |
| P31HG2 | 1.00 |
| P31HG3 | 1.00 |
| P31HD2 | 1.00 |
| P31HD3 | 1.00 |
| P31HB3 | 1.00 |
| V32H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO31 | HA | 1.00 | 0.002 | 1.00 | 0.73 |
| PRO31 | HB2 | 1.00 | 0.059 | 0.00 | 0.00 |
| PRO31 | HB3 | 1.00 | 0.005 | 1.00 | 6.97 |
| PRO31 | HG2 | 1.00 | 0.063 | 0.00 | 0.00 |
| PRO31 | HG3 | 1.00 | 0.005 | 1.00 | 1.67 |
| PRO31 | HD2 | 1.00 | 0.033 | 0.70 | 0.00 |
| PRO31 | HD3 | 1.00 | 0.034 | 0.60 | 0.00 |
| VAL32 | H | 1.00 | 0.001 | 1.00 | -258788.00 |

3.31.8 Detailed Probabilities of PRO31HG2:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO31 | 0.57 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P31HA | 1.00 |
| P31HB2 | 1.00 |
| P31HB3 | 1.00 |
| P31HG3 | 1.00 |
| P31HD2 | 1.00 |
| P31HD3 | 1.00 |
| P31HG2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO31 | HA | 1.00 | 0.006 | 1.00 | 0.37 |
| PRO31 | HB2 | 1.00 | 0.043 | 0.00 | 0.00 |
| PRO31 | HB3 | 1.00 | 0.007 | 1.00 | 0.97 |
| PRO31 | HG2 | 1.00 | 0.024 | 1.00 | 31.34 |
| PRO31 | HG3 | 1.00 | 0.002 | 1.00 | 3.30 |
| PRO31 | HD2 | 1.00 | 0.052 | 0.00 | 0.00 |
| PRO31 | HD3 | 1.00 | 0.055 | 0.00 | 0.00 |

3.31.9 Detailed Probabilities of PRO31HG3:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO31 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P31HA | 1.00 |
| P31HB2 | 1.00 |
| P31HB3 | 1.00 |
| P31HG2 | 1.00 |
| P31HD2 | 1.00 |
| P31HD3 | 1.00 |
| P31HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO31 | HA | 1.00 | 0.002 | 1.00 | 0.40 |
| PRO31 | HB2 | 1.00 | 0.092 | 0.00 | 0.00 |
| PRO31 | HB3 | 1.00 | 0.018 | 1.00 | 1.37 |
| PRO31 | HG2 | 1.00 | 0.081 | 0.00 | 0.00 |
| PRO31 | HG3 | 1.00 | 0.025 | 1.00 | 12.54 |
| PRO31 | HD2 | 1.00 | 0.007 | 1.00 | 0.97 |
| PRO31 | HD3 | 1.00 | 0.008 | 1.00 | 0.80 |

3.31.10 Detailed Probabilities of PRO31HD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS30 | 1.00 | 1.00 |
| PRO31 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K30H | 0.99 |
| K30HB3 | 0.99 |
| K30HA | 1.00 |
| K30HB2 | 0.99 |
| P31HA | 1.00 |
| P31HB2 | 1.00 |
| P31HB3 | 1.00 |
| P31HG2 | 1.00 |
| P31HG3 | 1.00 |
| P31HD3 | 1.00 |
| P31HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS30 | HA | 1.00 | 0.008 | 1.00 | 1.58 |
| LYS30 | HB2 | 0.99 | 0.007 | 1.00 | 0.42 |
| LYS30 | HB3 | 0.99 | 0.006 | 1.00 | 0.20 |
| LYS30 | H | 0.99 | 0.009 | 1.00 | -149310.00 |
| LYS30 | HG2 | 0.93 | 0.003 | 1.00 | 0.11 |
| LYS30 | HG3 | 0.92 | 0.003 | 1.00 | 0.11 |
| LYS30 | HD2 | 0.66 | 0.006 | 1.00 | 0.06 |
| LYS30 | HD3 | 0.66 | 0.001 | 1.00 | 0.11 |
| PRO31 | HA | 1.00 | 0.010 | 1.00 | 0.15 |
| PRO31 | HB2 | 1.00 | 0.019 | 1.00 | 0.62 |
| PRO31 | HB3 | 1.00 | 0.001 | 1.00 | 0.25 |
| PRO31 | HG2 | 1.00 | 0.000 | 1.00 | 0.93 |
| PRO31 | HG3 | 1.00 | 0.002 | 1.00 | 0.75 |
| PRO31 | HD2 | 1.00 | 0.002 | 1.00 | 5.09 |
| PRO31 | HD3 | 1.00 | 0.011 | 1.00 | 4.51 |

3.31.11 Detailed Probabilities of PRO31HD3:

Overall probability: 0.847

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS30 | 0.83 | 1.00 |
| PRO31 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K30HB3 | 1.00 |
| K30HA | 1.00 |
| K30HB2 | 1.00 |
| K30H | 0.99 |
| P31HA | 1.00 |
| P31HB2 | 1.00 |
| P31HB3 | 1.00 |
| P31HG2 | 1.00 |
| P31HG3 | 1.00 |
| P31HD2 | 1.00 |
| P31HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS30 | HA | 1.00 | 0.002 | 1.00 | 0.94 |
| LYS30 | HB2 | 1.00 | 0.000 | 1.00 | 0.74 |
| LYS30 | HB3 | 1.00 | 0.000 | 1.00 | 0.33 |
| LYS30 | H | 0.99 | 0.081 | 0.01 | 0.00 |
| LYS30 | HG2 | 0.79 | 0.000 | 1.00 | 0.16 |
| LYS30 | HG3 | 0.78 | 0.000 | 1.00 | 0.16 |
| PRO31 | HA | 1.00 | 0.003 | 1.00 | 0.14 |
| PRO31 | HB2 | 1.00 | 0.010 | 1.00 | 0.52 |
| PRO31 | HB3 | 1.00 | 0.009 | 1.00 | 0.36 |
| PRO31 | HG2 | 1.00 | 0.001 | 1.00 | 0.99 |
| PRO31 | HG3 | 1.00 | 0.041 | 0.00 | 0.00 |
| PRO31 | HD2 | 1.00 | 0.009 | 1.00 | 4.34 |
| PRO31 | HD3 | 1.00 | 0.022 | 1.00 | 5.59 |

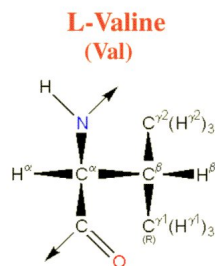
3.32 VAL(32)

Figure 22: Image from the BMRB

Residue probability: 0.880

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 173.962 | 175.682 | 2.367 | 0.000 | 0.000 |
| CA 3.32.1 | 62.771 | 62.613 | 4.828 | 0.701 | 1.000 |
| CB 3.32.2 | 30.256 | 32.918 | 4.591 | 0.667 | 1.000 |
| CG1 3.32.3 | 21.642 | 21.563 | 2.746 | 1.000 | 1.000 |
| CG2 3.32.4 | 21.562 | 21.368 | 2.801 | 1.000 | 1.000 |
| N 3.32.5 | 121.796 | 121.057 | 5.832 | 1.000 | 1.000 |
| HA 3.32.6 | 4.218 | 4.178 | 0.599 | 0.601 | 1.000 |
| HB 3.32.7 | 2.110 | 1.980 | 0.322 | 0.833 | 1.000 |
| HG1 3.32.8 | 0.682 | 0.816 | 0.264 | 1.000 | 1.000 |
| HG2 3.32.9 | 0.680 | 0.803 | 0.504 | 1.000 | 1.000 |
| H 3.32.10 | 7.872 | 8.311 | 0.669 | 1.000 | 1.000 |

3.32.1 Detailed Probabilities of VAL32CA:

Overall probability: 0.701

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO31 | 0.34 | 1.00 |
| VAL32 | 1.00 | 1.00 |
| LEU33 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P31HB2 | 0.99 |
| P31HA | 1.00 |
| V32HG11 | 1.00 |
| V32HG21 | 1.00 |
| V32H | 1.00 |
| V32HB | 1.00 |
| V32HA | 1.00 |
| L33H | 1.00 |
| L33HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO31 | HA | 1.00 | 0.118 | 0.00 | 0.00 |
| PRO31 | HB2 | 0.99 | 0.214 | 0.01 | 0.00 |
| PRO31 | HG2 | 0.65 | 0.007 | 1.00 | 0.33 |
| VAL32 | HA | 1.00 | 0.000 | 1.00 | 7.43 |
| VAL32 | HB | 1.00 | 0.004 | 1.00 | 0.33 |
| VAL32 | HG11 | 1.00 | 0.005 | 1.00 | 2.62 |
| VAL32 | HG21 | 1.00 | 0.003 | 1.00 | 2.62 |
| VAL32 | H | 1.00 | 0.001 | 1.00 | 0.23 |
| LEU33 | HA | 1.00 | 0.330 | 0.00 | 0.00 |
| LEU33 | H | 1.00 | 0.001 | 1.00 | 0.21 |

3.32.2 Detailed Probabilities of VAL32CB:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL32 | 0.60 | 1.00 |
| LEU33 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V32HA | 1.00 |
| V32HG11 | 1.00 |
| V32HG21 | 1.00 |
| V32H | 1.00 |
| V32HB | 1.00 |
| L33H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL32 | HA | 1.00 | 1.308 | 0.00 | 0.00 |
| VAL32 | HB | 1.00 | 0.487 | 0.00 | 0.00 |
| VAL32 | HG11 | 1.00 | 0.005 | 1.00 | 2.28 |
| VAL32 | HG21 | 1.00 | 0.003 | 1.00 | 2.28 |
| VAL32 | H | 1.00 | 0.002 | 1.00 | 0.42 |
| LEU33 | H | 1.00 | 0.002 | 1.00 | 1.08 |

3.32.3 Detailed Probabilities of VAL32CG1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL32 | 1.00 | 1.00 |
| LEU33 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V32HA | 1.00 |
| V32HG12 | 1.00 |
| V32HG21 | 1.00 |
| V32H | 1.00 |
| V32HB | 1.00 |
| L33H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL32 | HA | 1.00 | 0.000 | 1.00 | 2.24 |
| VAL32 | HB | 1.00 | 0.003 | 1.00 | 2.41 |
| VAL32 | HG11 | 1.00 | 0.006 | 1.00 | 69.71 |
| VAL32 | HG21 | 1.00 | 0.004 | 1.00 | 69.71 |
| VAL32 | H | 1.00 | 0.000 | 1.00 | 0.66 |
| LEU33 | H | 0.98 | 0.002 | 1.00 | 1.53 |

3.32.4 Detailed Probabilities of VAL32CG2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL32 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V32HA | 1.00 |
| V32HG11 | 1.00 |
| V32HG22 | 1.00 |
| V32H | 1.00 |
| V32HB | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL32 | HA | 1.00 | 0.000 | 1.00 | 2.24 |
| VAL32 | HB | 1.00 | 0.003 | 1.00 | 2.41 |
| VAL32 | HG11 | 1.00 | 0.006 | 1.00 | 69.71 |
| VAL32 | HG21 | 1.00 | 0.004 | 1.00 | 69.71 |
| VAL32 | H | 1.00 | 0.000 | 1.00 | 0.66 |

3.32.5 Detailed Probabilities of VAL32N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO31 | 1.00 | 1.00 |
| VAL32 | 1.00 | 1.00 |
| LEU33 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P31HB2 | 1.00 |
| P31HA | 1.00 |
| P31HB3 | 1.00 |
| V32HA | 1.00 |
| V32HG11 | 1.00 |
| V32HG21 | 1.00 |
| V32HB | 1.00 |
| V32H | 1.00 |
| L33H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO31 | HA | 1.00 | 0.001 | 1.00 | -1794731.00 |
| PRO31 | HB2 | 1.00 | 0.001 | 1.00 | -377089.00 |
| PRO31 | HB3 | 1.00 | 0.001 | 1.00 | -258788.00 |
| PRO31 | HG2 | 0.89 | 0.007 | 1.00 | -631385.00 |
| PRO31 | HG3 | 0.70 | 0.009 | 1.00 | -95436.00 |
| VAL32 | HA | 1.00 | 0.007 | 1.00 | -301691.00 |
| VAL32 | HB | 1.00 | 0.004 | 1.00 | -631385.00 |
| VAL32 | HG11 | 1.00 | 0.005 | 1.00 | -935676.00 |
| VAL32 | HG21 | 1.00 | 0.003 | 1.00 | -935676.00 |
| VAL32 | H | 1.00 | 0.004 | 1.00 | -4403788.00 |
| LEU33 | H | 1.00 | 0.003 | 1.00 | -462997.00 |
| LEU33 | HA | 0.94 | 0.028 | 1.00 | -125171.00 |

3.32.6 Detailed Probabilities of VAL32HA:

Overall probability: 0.601

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO31 | 0.34 | 1.00 |
| VAL32 | 0.80 | 1.00 |
| LEU33 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P31HB2 | 0.99 |
| P31HA | 1.00 |
| V32HG11 | 1.00 |
| V32HG21 | 1.00 |
| V32H | 1.00 |
| V32HB | 1.00 |
| V32HA | 1.00 |
| L33H | 1.00 |
| L33HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO31 | HA | 1.00 | 0.119 | 0.00 | 0.00 |
| PRO31 | HB2 | 0.99 | 0.044 | 0.01 | 0.00 |
| PRO31 | HG2 | 0.65 | 0.027 | 1.00 | 0.69 |
| VAL32 | HA | 1.00 | 0.000 | 1.00 | 7.43 |
| VAL32 | HB | 1.00 | 1.308 | 0.00 | 0.00 |
| VAL32 | HG11 | 1.00 | 0.000 | 1.00 | 2.24 |
| VAL32 | HG21 | 1.00 | 0.000 | 1.00 | 2.24 |
| VAL32 | H | 1.00 | 0.007 | 1.00 | -301691.00 |
| LEU33 | HA | 1.00 | 0.149 | 0.00 | 0.00 |
| LEU33 | H | 1.00 | 0.001 | 1.00 | -379454.00 |

3.32.7 Detailed Probabilities of VAL32HB:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL32 | 0.80 | 1.00 |
| LEU33 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V32HA | 1.00 |
| V32HG11 | 1.00 |
| V32HG21 | 1.00 |
| V32H | 1.00 |
| V32HB | 1.00 |
| L33H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL32 | HA | 1.00 | 0.004 | 1.00 | 0.33 |
| VAL32 | HB | 1.00 | 0.487 | 0.00 | 0.00 |
| VAL32 | HG11 | 1.00 | 0.003 | 1.00 | 2.41 |
| VAL32 | HG21 | 1.00 | 0.003 | 1.00 | 2.41 |
| VAL32 | H | 1.00 | 0.004 | 1.00 | -631385.00 |
| LEU33 | H | 1.00 | 0.002 | 1.00 | -2403188.00 |

3.32.8 Detailed Probabilities of VAL32HG11:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL32 | 1.00 | 1.00 |
| LEU33 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V32HA | 1.00 |
| V32HG12 | 1.00 |
| V32HG21 | 1.00 |
| V32H | 1.00 |
| V32HB | 1.00 |
| L33H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL32 | HA | 1.00 | 0.005 | 1.00 | 2.62 |
| VAL32 | HB | 1.00 | 0.005 | 1.00 | 2.28 |
| VAL32 | HG11 | 1.00 | 0.006 | 1.00 | 69.71 |
| VAL32 | HG21 | 1.00 | 0.006 | 1.00 | 69.71 |
| VAL32 | H | 1.00 | 0.005 | 1.00 | -935676.00 |
| LEU33 | H | 0.98 | 0.007 | 1.00 | -2828770.00 |

3.32.9 Detailed Probabilities of VAL32HG21:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL32 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V32HA | 1.00 |
| V32HG11 | 1.00 |
| V32HG22 | 1.00 |
| V32H | 1.00 |
| V32HB | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL32 | HA | 1.00 | 0.003 | 1.00 | 2.62 |
| VAL32 | HB | 1.00 | 0.003 | 1.00 | 2.28 |
| VAL32 | HG11 | 1.00 | 0.004 | 1.00 | 69.71 |
| VAL32 | HG21 | 1.00 | 0.004 | 1.00 | 69.71 |
| VAL32 | H | 1.00 | 0.003 | 1.00 | -935676.00 |

3.32.10 Detailed Probabilities of VAL32H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO31 | 1.00 | 1.00 |
| VAL32 | 1.00 | 1.00 |
| LEU33 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P31HB2 | 1.00 |
| P31HA | 1.00 |
| P31HB3 | 1.00 |
| V32HA | 1.00 |
| V32HG11 | 1.00 |
| V32HG21 | 1.00 |
| V32HB | 1.00 |
| V32H | 1.00 |
| L33H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO31 | HA | 1.00 | 0.003 | 1.00 | 1.69 |
| PRO31 | HB2 | 1.00 | 0.005 | 1.00 | 0.35 |
| PRO31 | HB3 | 1.00 | 0.007 | 1.00 | 0.25 |
| PRO31 | HG2 | 0.89 | 0.001 | 1.00 | 0.05 |
| PRO31 | HG3 | 0.70 | 0.004 | 1.00 | 0.06 |
| PRO31 | HD2 | 0.63 | 0.019 | 1.00 | 0.05 |
| VAL32 | HA | 1.00 | 0.001 | 1.00 | 0.23 |
| VAL32 | HB | 1.00 | 0.002 | 1.00 | 0.42 |
| VAL32 | HG11 | 1.00 | 0.000 | 1.00 | 0.66 |
| VAL32 | HG21 | 1.00 | 0.000 | 1.00 | 0.66 |
| VAL32 | H | 1.00 | 0.004 | 1.00 | -4403788.00 |
| LEU33 | H | 1.00 | 0.002 | 1.00 | -297883.00 |

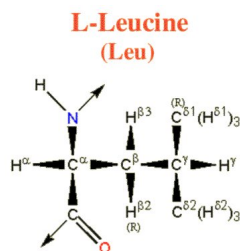
3.33 LEU(33)

Figure 23: Image from the BMRB

Residue probability: 0.665

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 177.525 | 177.056 | 1.929 | 0.000 | 0.000 |
| CA 3.33.1 | 54.256 | 55.735 | 3.802 | 0.701 | 1.000 |
| CB 3.33.2 | 43.015 | 42.389 | 3.750 | 0.625 | 1.000 |
| CG 3.33.3 | 27.248 | 26.892 | 3.086 | 0.378 | 1.000 |
| CD1 3.33.4 | 27.157 | 24.837 | 3.657 | 0.829 | 1.000 |
| CD2 3.33.5 | 23.739 | 24.201 | 3.117 | 0.429 | 1.000 |
| N 3.33.6 | 118.002 | 121.785 | 4.943 | 0.993 | 1.000 |
| HA 3.33.7 | 4.635 | 4.315 | 0.840 | 0.818 | 1.000 |
| HB2 3.33.8 | 1.648 | 1.601 | 0.373 | 0.725 | 1.000 |
| HB3 3.33.9 | 1.521 | 1.508 | 0.398 | 0.625 | 1.000 |
| HG 3.33.10 | 1.596 | 1.510 | 0.340 | 0.438 | 1.000 |
| HD1 3.33.11 | 0.852 | 0.739 | 0.294 | 0.668 | 1.000 |
| HD2 3.33.12 | 0.911 | 0.727 | 0.421 | 0.414 | 1.000 |
| H 3.33.13 | 7.566 | 8.237 | 0.647 | 1.000 | 1.000 |

3.33.1 Detailed Probabilities of LEU33CA:

Overall probability: 0.701

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL32 | 0.00 | 1.00 |
| LEU33 | 0.72 | 1.00 |
| GLU34 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V32HA | 1.00 |
| L33HB2 | 1.00 |
| L33HB3 | 1.00 |
| L33HG | 1.00 |
| L33HD11 | 0.99 |
| L33HD21 | 0.99 |
| L33H | 1.00 |
| L33HA | 1.00 |
| E34HA | 1.00 |
| E34H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL32 | HA | 1.00 | 0.149 | 0.00 | 0.00 |
| LEU33 | HA | 1.00 | 0.025 | 1.00 | 10.54 |
| LEU33 | HB2 | 1.00 | 0.001 | 1.00 | 0.31 |
| LEU33 | HB3 | 1.00 | 0.001 | 1.00 | 0.52 |
| LEU33 | HG | 1.00 | 0.053 | 0.00 | 0.00 |
| LEU33 | HD11 | 0.99 | 0.057 | 0.01 | 0.00 |
| LEU33 | HD21 | 0.99 | 0.002 | 1.00 | 1.34 |
| LEU33 | H | 1.00 | 0.001 | 1.00 | 0.37 |
| GLU34 | HA | 1.00 | 0.017 | 1.00 | 0.06 |
| GLU34 | H | 1.00 | 0.016 | 1.00 | 0.41 |

3.33.2 Detailed Probabilities of LEU33CB:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU33 | 0.71 | 1.00 |
| GLU34 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L33HA | 1.00 |
| L33HB3 | 1.00 |
| L33HG | 1.00 |
| L33HD11 | 1.00 |
| L33HD21 | 1.00 |
| L33H | 1.00 |
| L33HB2 | 1.00 |
| E34H | 1.00 |

NOESY contacts detailed probability

3.33 LEU(33)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU33 | HA | 1.00 | 0.003 | 1.00 | 0.32 |
| LEU33 | HB2 | 1.00 | 0.006 | 1.00 | 2.17 |
| LEU33 | HB3 | 1.00 | 0.002 | 1.00 | 1.73 |
| LEU33 | HG | 1.00 | 0.046 | 0.00 | 0.00 |
| LEU33 | HD11 | 1.00 | 0.017 | 1.00 | 0.55 |
| LEU33 | HD21 | 1.00 | 0.042 | 0.00 | 0.00 |
| LEU33 | H | 1.00 | 0.002 | 1.00 | 0.35 |
| GLU34 | H | 1.00 | 1.433 | 0.00 | 0.00 |

3.33.3 Detailed Probabilities of LEU33CG:

Overall probability: 0.378

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU33 | 0.43 | 1.00 |
| GLU34 | 0.02 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L33HA | 1.00 |
| L33HB2 | 1.00 |
| L33HB3 | 1.00 |
| L33HD11 | 1.00 |
| L33HD21 | 1.00 |
| L33H | 1.00 |
| L33HG | 1.00 |
| E34H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU33 | HA | 1.00 | 0.005 | 1.00 | 0.17 |
| LEU33 | HB2 | 1.00 | 0.329 | 0.00 | 0.00 |
| LEU33 | HB3 | 1.00 | 0.202 | 0.00 | 0.00 |
| LEU33 | HG | 1.00 | 0.277 | 0.00 | 0.00 |
| LEU33 | HD11 | 1.00 | 0.003 | 1.00 | 2.31 |
| LEU33 | HD21 | 1.00 | 0.062 | 0.00 | 0.00 |
| LEU33 | H | 1.00 | 0.002 | 1.00 | 0.21 |
| GLU34 | H | 0.98 | 1.433 | 0.02 | 0.00 |

3.33.4 Detailed Probabilities of LEU33CD1:

Overall probability: 0.829

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU33 | 0.83 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L33HA | 0.99 |
| L33HB2 | 1.00 |
| L33HB3 | 1.00 |
| L33HG | 1.00 |
| L33HD12 | 1.00 |
| L33HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU33 | HA | 0.99 | 0.004 | 1.00 | 0.41 |
| LEU33 | HB2 | 1.00 | 0.032 | 0.80 | 0.00 |
| LEU33 | HB3 | 1.00 | 0.011 | 1.00 | 0.78 |
| LEU33 | HG | 1.00 | 0.020 | 1.00 | 3.39 |
| LEU33 | HD11 | 1.00 | 0.007 | 1.00 | 32.08 |
| LEU33 | HD21 | 1.00 | 0.066 | 0.00 | 0.00 |
| LEU33 | H | 0.86 | 0.005 | 1.00 | 0.30 |

3.33.5 Detailed Probabilities of LEU33CD2:

Overall probability: 0.429

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU33 | 0.43 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L33HA | 0.99 |
| L33HB2 | 1.00 |
| L33HB3 | 1.00 |
| L33HG | 1.00 |
| L33HD11 | 1.00 |
| L33HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU33 | HA | 0.99 | 0.003 | 1.00 | 1.99 |
| LEU33 | HB2 | 1.00 | 0.045 | 0.00 | 0.00 |
| LEU33 | HB3 | 1.00 | 0.082 | 0.00 | 0.00 |
| LEU33 | HG | 1.00 | 0.007 | 1.00 | 2.25 |
| LEU33 | HD11 | 1.00 | 0.136 | 0.00 | 0.00 |
| LEU33 | HD21 | 1.00 | 0.195 | 0.00 | 0.00 |
| LEU33 | H | 0.85 | 0.001 | 1.00 | 0.22 |

3.33.6 Detailed Probabilities of LEU33N:

Overall probability: 0.993

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL32 | 1.00 | 1.00 |
| LEU33 | 0.98 | 1.00 |
| GLU34 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V32HG11 | 0.98 |
| V32HB | 1.00 |
| V32H | 1.00 |
| V32HA | 1.00 |
| L33HA | 1.00 |
| L33HB2 | 1.00 |
| L33HB3 | 1.00 |
| L33HG | 1.00 |
| L33H | 1.00 |
| E34H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL32 | HA | 1.00 | 0.001 | 1.00 | -379454.00 |
| VAL32 | HB | 1.00 | 0.002 | 1.00 | -2403188.00 |
| VAL32 | HG11 | 0.98 | 0.007 | 1.00 | -2828770.00 |
| VAL32 | H | 1.00 | 0.002 | 1.00 | -297883.00 |
| VAL32 | HG21 | 0.94 | 0.005 | 1.00 | -2828770.00 |
| LEU33 | HA | 1.00 | 0.007 | 1.00 | -548309.00 |
| LEU33 | HB2 | 1.00 | 0.021 | 1.00 | -1476307.00 |
| LEU33 | HB3 | 1.00 | 0.010 | 1.00 | -758690.00 |
| LEU33 | HG | 1.00 | 0.031 | 0.90 | 0.00 |
| LEU33 | H | 1.00 | 0.001 | 1.00 | -10702306.00 |
| LEU33 | HD21 | 0.87 | 0.019 | 1.00 | -450382.00 |
| GLU34 | H | 1.00 | 0.005 | 1.00 | -550022.00 |
| GLU34 | HA | 0.90 | 0.011 | 1.00 | -263139.00 |
| GLU34 | HB2 | 0.55 | 0.006 | 1.00 | -201773.00 |

3.33.7 Detailed Probabilities of LEU33HA:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL32 | 0.50 | 1.00 |
| LEU33 | 1.00 | 1.00 |
| GLU34 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V32HA | 1.00 |
| L33HB2 | 1.00 |
| L33HB3 | 1.00 |
| L33HG | 1.00 |
| L33HD11 | 0.99 |
| L33HD21 | 0.99 |
| L33H | 1.00 |
| L33HA | 1.00 |
| E34HA | 1.00 |
| E34H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL32 | HA | 1.00 | 0.330 | 0.00 | 0.00 |
| VAL32 | H | 0.94 | 0.028 | 1.00 | -125171.00 |
| LEU33 | HA | 1.00 | 0.025 | 1.00 | 10.54 |
| LEU33 | HB2 | 1.00 | 0.003 | 1.00 | 0.32 |
| LEU33 | HB3 | 1.00 | 0.004 | 1.00 | 0.41 |
| LEU33 | HG | 1.00 | 0.005 | 1.00 | 0.17 |
| LEU33 | HD11 | 0.99 | 0.004 | 1.00 | 0.41 |
| LEU33 | HD21 | 0.99 | 0.003 | 1.00 | 1.99 |
| LEU33 | H | 1.00 | 0.007 | 1.00 | -548309.00 |
| GLU34 | HA | 1.00 | 0.164 | 0.00 | 0.00 |
| GLU34 | H | 1.00 | 0.004 | 1.00 | -632238.00 |

3.33.8 Detailed Probabilities of LEU33HB2:

Overall probability: 0.725

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU33 | 0.69 | 1.00 |
| GLU34 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L33HA | 1.00 |
| L33HB3 | 1.00 |
| L33HG | 1.00 |
| L33HD11 | 1.00 |
| L33HD21 | 1.00 |
| L33H | 1.00 |
| L33HB2 | 1.00 |
| E34H | 1.00 |

NOESY contacts detailed probability

3.33 LEU(33)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU33 | HA | 1.00 | 0.001 | 1.00 | 0.31 |
| LEU33 | HB2 | 1.00 | 0.006 | 1.00 | 2.17 |
| LEU33 | HB3 | 1.00 | 0.008 | 1.00 | 1.97 |
| LEU33 | HG | 1.00 | 0.329 | 0.00 | 0.00 |
| LEU33 | HD11 | 1.00 | 0.032 | 0.80 | 0.00 |
| LEU33 | HD21 | 1.00 | 0.045 | 0.00 | 0.00 |
| LEU33 | H | 1.00 | 0.021 | 1.00 | -1476307.00 |
| GLU34 | H | 1.00 | 0.018 | 1.00 | -204054.00 |

3.33.9 Detailed Probabilities of LEU33HB3:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU33 | 0.57 | 1.00 |
| GLU34 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L33HA | 1.00 |
| L33HB2 | 1.00 |
| L33HG | 1.00 |
| L33HD11 | 1.00 |
| L33HD21 | 1.00 |
| L33H | 1.00 |
| L33HB3 | 1.00 |
| E34H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU33 | HA | 1.00 | 0.001 | 1.00 | 0.52 |
| LEU33 | HB2 | 1.00 | 0.002 | 1.00 | 1.73 |
| LEU33 | HB3 | 1.00 | 0.099 | 0.00 | 0.00 |
| LEU33 | HG | 1.00 | 0.202 | 0.00 | 0.00 |
| LEU33 | HD11 | 1.00 | 0.011 | 1.00 | 0.78 |
| LEU33 | HD21 | 1.00 | 0.082 | 0.00 | 0.00 |
| LEU33 | H | 1.00 | 0.010 | 1.00 | -758690.00 |
| GLU34 | H | 1.00 | 0.005 | 1.00 | -179064.00 |

3.33.10 Detailed Probabilities of LEU33HG:

Overall probability: 0.438

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU33 | 0.41 | 1.00 |
| GLU34 | 0.60 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L33HA | 1.00 |
| L33HB2 | 1.00 |
| L33HB3 | 1.00 |
| L33HD11 | 1.00 |
| L33HD21 | 1.00 |
| L33H | 1.00 |
| L33HG | 1.00 |
| E34H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU33 | HA | 1.00 | 0.053 | 0.00 | 0.00 |
| LEU33 | HB2 | 1.00 | 0.046 | 0.00 | 0.00 |
| LEU33 | HB3 | 1.00 | 0.060 | 0.00 | 0.00 |
| LEU33 | HG | 1.00 | 0.277 | 0.00 | 0.00 |
| LEU33 | HD11 | 1.00 | 0.020 | 1.00 | 3.39 |
| LEU33 | HD21 | 1.00 | 0.007 | 1.00 | 2.25 |
| LEU33 | H | 1.00 | 0.031 | 0.90 | 0.00 |
| GLU34 | H | 0.98 | 0.034 | 0.60 | 0.00 |

3.33.11 Detailed Probabilities of LEU33HD11:

Overall probability: 0.668

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU33 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L33HA | 0.99 |
| L33HB2 | 1.00 |
| L33HB3 | 1.00 |
| L33HG | 1.00 |
| L33HD12 | 1.00 |
| L33HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU33 | HA | 0.99 | 0.057 | 0.01 | 0.00 |
| LEU33 | HB2 | 1.00 | 0.017 | 1.00 | 0.55 |
| LEU33 | HB3 | 1.00 | 0.028 | 1.00 | 0.71 |
| LEU33 | HG | 1.00 | 0.003 | 1.00 | 2.31 |
| LEU33 | HD11 | 1.00 | 0.007 | 1.00 | 32.08 |
| LEU33 | HD21 | 1.00 | 0.136 | 0.00 | 0.00 |

3.33.12 Detailed Probabilities of LEU33HD21:

Overall probability: 0.414

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU33 | 0.41 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L33HA | 0.99 |
| L33HB2 | 1.00 |
| L33HB3 | 1.00 |
| L33HG | 1.00 |
| L33HD11 | 1.00 |
| L33HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU33 | HA | 0.99 | 0.002 | 1.00 | 1.34 |
| LEU33 | HB2 | 1.00 | 0.042 | 0.00 | 0.00 |
| LEU33 | HB3 | 1.00 | 0.031 | 0.90 | 0.00 |
| LEU33 | HG | 1.00 | 0.062 | 0.00 | 0.00 |
| LEU33 | HD11 | 1.00 | 0.066 | 0.00 | 0.00 |
| LEU33 | HD21 | 1.00 | 0.195 | 0.00 | 0.00 |
| LEU33 | H | 0.85 | 0.019 | 1.00 | -450382.00 |

3.33.13 Detailed Probabilities of LEU33H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL32 | 1.00 | 1.00 |
| LEU33 | 1.00 | 1.00 |
| GLU34 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V32HG11 | 0.98 |
| V32HB | 1.00 |
| V32H | 1.00 |
| V32HA | 1.00 |
| L33HA | 1.00 |
| L33HB2 | 1.00 |
| L33HB3 | 1.00 |
| L33HG | 1.00 |
| L33H | 1.00 |
| E34H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL32 | HA | 1.00 | 0.001 | 1.00 | 0.21 |
| VAL32 | HB | 1.00 | 0.002 | 1.00 | 1.08 |
| VAL32 | HG11 | 0.98 | 0.002 | 1.00 | 1.53 |
| VAL32 | H | 1.00 | 0.003 | 1.00 | -462997.00 |
| VAL32 | HG21 | 0.94 | 0.002 | 1.00 | 1.53 |
| LEU33 | HA | 1.00 | 0.001 | 1.00 | 0.37 |
| LEU33 | HB2 | 1.00 | 0.002 | 1.00 | 0.35 |
| LEU33 | HB3 | 1.00 | 0.001 | 1.00 | 0.28 |
| LEU33 | HG | 1.00 | 0.002 | 1.00 | 0.21 |
| LEU33 | H | 1.00 | 0.001 | 1.00 | -10702306.00 |
| LEU33 | HD11 | 0.88 | 0.005 | 1.00 | 0.30 |
| LEU33 | HD21 | 0.87 | 0.001 | 1.00 | 0.22 |
| GLU34 | H | 1.00 | 0.002 | 1.00 | -557139.00 |

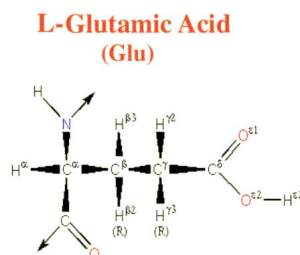
3.34 GLU(34)

Figure 24: Image from the BMRB

Residue probability: 0.640

Residue probability confidence: 0.811

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | NA | – | – | 0.000 | 0.000 |
| CA 3.34.1 | 60.709 | 57.442 | 3.837 | 0.500 | 0.889 |
| CB 3.34.2 | 29.929 | 30.185 | 4.018 | 0.667 | 0.750 |
| CG 3.34.3 | 36.955 | 36.085 | 1.533 | 0.667 | 0.750 |
| N 3.34.4 | 119.011 | 120.574 | 4.837 | 0.800 | 0.917 |
| HA 3.34.5 | 4.052 | 4.245 | 0.429 | 1.000 | 0.889 |
| HB2 3.34.6 | 2.325 | 2.021 | 0.233 | 0.667 | 0.750 |
| HB3 3.34.7 | 2.323 | 1.994 | 0.244 | 0.667 | 0.750 |
| HG2 3.34.8 | 2.234 | 2.258 | 0.226 | 0.333 | 0.750 |
| HG3 3.34.9 | 2.235 | 2.233 | 0.232 | 0.333 | 0.750 |
| H 3.34.10 | 8.997 | 8.332 | 0.601 | 0.771 | 0.917 |
| HE2 | NA | – | – | 0.000 | 0.000 |

3.34.1 Detailed Probabilities of GLU34CA:

Overall probability: 0.500

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU33 | 0.00 | 1.00 |
| GLU34 | 0.67 | 1.00 |
| THR35 | 0.00 | 0.50 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L33HA | 1.00 |
| E34HB2 | 1.00 |
| E34HB3 | 1.00 |
| E34HG2 | 1.00 |
| E34HG3 | 1.00 |
| E34H | 1.00 |
| E34HA | 1.00 |
| T35H | 1.00 |
| T35HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU33 | HA | 1.00 | 0.164 | 0.00 | 0.00 |
| GLU34 | HA | 1.00 | 0.000 | 1.00 | 5.95 |
| GLU34 | HB2 | 1.00 | 0.010 | 1.00 | 1.32 |
| GLU34 | HB3 | 1.00 | 0.008 | 1.00 | 1.32 |
| GLU34 | HG2 | 1.00 | 0.081 | 0.00 | 0.00 |
| GLU34 | HG3 | 1.00 | 0.080 | 0.00 | 0.00 |
| GLU34 | H | 1.00 | 0.009 | 1.00 | 0.64 |
| THR35 | HA | 1.00 | 0.049 | 0.00 | 0.00 |

3.34.2 Detailed Probabilities of GLU34CB:

Overall probability: 0.667

Overall confidence: 0.750

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU34 | 0.67 | 0.86 |
| THR35 | 0.00 | 0.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E34HA | 1.00 |
| E34HB3 | 1.00 |
| E34HG2 | 1.00 |
| E34HG3 | 1.00 |
| E34H | 1.00 |
| E34HE2 | 1.00 |
| E34HB2 | 1.00 |
| T35H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU34 | HA | 1.00 | 0.002 | 1.00 | 0.74 |
| GLU34 | HB2 | 1.00 | 0.004 | 1.00 | 9.85 |
| GLU34 | HB3 | 1.00 | 0.002 | 1.00 | 9.85 |
| GLU34 | HG2 | 1.00 | 0.087 | 0.00 | 0.00 |
| GLU34 | HG3 | 1.00 | 0.086 | 0.00 | 0.00 |
| GLU34 | H | 1.00 | 0.006 | 1.00 | 0.23 |

3.34.3 Detailed Probabilities of GLU34CG:

Overall probability: 0.667

Overall confidence: 0.750

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU34 | 0.67 | 0.86 |
| THR35 | 0.00 | 0.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E34HA | 1.00 |
| E34HB2 | 1.00 |
| E34HB3 | 1.00 |
| E34HG3 | 1.00 |
| E34H | 1.00 |
| E34HE2 | 1.00 |
| E34HG2 | 1.00 |
| T35H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU34 | HA | 1.00 | 0.030 | 1.00 | 1.51 |
| GLU34 | HB2 | 1.00 | 0.105 | 0.00 | 0.00 |
| GLU34 | HB3 | 1.00 | 0.103 | 0.00 | 0.00 |
| GLU34 | HG2 | 1.00 | 0.014 | 1.00 | 180.23 |
| GLU34 | HG3 | 1.00 | 0.015 | 1.00 | 180.23 |
| GLU34 | H | 1.00 | 0.008 | 1.00 | 0.25 |

3.34.4 Detailed Probabilities of GLU34N:

Overall probability: 0.800

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU33 | 0.93 | 1.00 |
| GLU34 | 0.67 | 1.00 |
| THR35 | 0.00 | 0.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L33HA | 1.00 |
| L33HB2 | 1.00 |
| L33HB3 | 1.00 |
| L33HG | 0.98 |
| L33H | 1.00 |
| E34HA | 1.00 |
| E34HB2 | 1.00 |
| E34HB3 | 1.00 |
| E34HG2 | 1.00 |
| E34HG3 | 1.00 |
| E34H | 1.00 |
| T35H | 1.00 |

NOESY contacts detailed probability

3.34 GLU(34)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU33 | HA | 1.00 | 0.004 | 1.00 | -632238.00 |
| LEU33 | HB2 | 1.00 | 0.018 | 1.00 | -204054.00 |
| LEU33 | HB3 | 1.00 | 0.005 | 1.00 | -179064.00 |
| LEU33 | HG | 0.98 | 0.034 | 0.60 | 0.00 |
| LEU33 | H | 1.00 | 0.002 | 1.00 | -557139.00 |
| LEU33 | HD21 | 0.58 | 0.019 | 1.00 | -187753.00 |
| GLU34 | HA | 1.00 | 0.000 | 1.00 | -1300126.00 |
| GLU34 | HB2 | 1.00 | 0.006 | 1.00 | -809996.00 |
| GLU34 | HB3 | 1.00 | 0.004 | 1.00 | -809996.00 |
| GLU34 | HG2 | 1.00 | 0.085 | 0.00 | 0.00 |
| GLU34 | HG3 | 1.00 | 0.084 | 0.00 | 0.00 |
| GLU34 | H | 1.00 | 0.005 | 1.00 | -2933712.00 |

3.34.5 Detailed Probabilities of GLU34HA:

Overall probability: 1.000

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU33 | 1.00 | 1.00 |
| GLU34 | 1.00 | 1.00 |
| THR35 | 1.00 | 0.50 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L33HA | 1.00 |
| E34HB2 | 1.00 |
| E34HB3 | 1.00 |
| E34HG2 | 1.00 |
| E34HG3 | 1.00 |
| E34H | 1.00 |
| E34HA | 1.00 |
| T35H | 1.00 |
| T35HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU33 | HA | 1.00 | 0.017 | 1.00 | 0.06 |
| LEU33 | H | 0.90 | 0.011 | 1.00 | -263139.00 |
| GLU34 | HA | 1.00 | 0.000 | 1.00 | 5.95 |
| GLU34 | HB2 | 1.00 | 0.002 | 1.00 | 0.74 |
| GLU34 | HB3 | 1.00 | 0.002 | 1.00 | 0.74 |
| GLU34 | HG2 | 1.00 | 0.030 | 1.00 | 1.51 |
| GLU34 | HG3 | 1.00 | 0.030 | 1.00 | 1.51 |
| GLU34 | H | 1.00 | 0.000 | 1.00 | -1300126.00 |
| THR35 | HA | 1.00 | 0.017 | 1.00 | 0.16 |

3.34.6 Detailed Probabilities of GLU34HB2:

Overall probability: 0.667

Overall confidence: 0.750

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU34 | 0.67 | 0.86 |
| THR35 | NaN | 0.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E34HA | 1.00 |
| E34HB3 | 1.00 |
| E34HG2 | 1.00 |
| E34HG3 | 1.00 |
| E34H | 1.00 |
| E34HE2 | 1.00 |
| E34HB2 | 1.00 |
| T35H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU34 | HA | 1.00 | 0.010 | 1.00 | 1.32 |
| GLU34 | HB2 | 1.00 | 0.004 | 1.00 | 9.85 |
| GLU34 | HB3 | 1.00 | 0.004 | 1.00 | 9.85 |
| GLU34 | HG2 | 1.00 | 0.105 | 0.00 | 0.00 |
| GLU34 | HG3 | 1.00 | 0.105 | 0.00 | 0.00 |
| GLU34 | H | 1.00 | 0.006 | 1.00 | -809996.00 |

3.34.7 Detailed Probabilities of GLU34HB3:

Overall probability: 0.667

Overall confidence: 0.750

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU34 | 0.67 | 0.86 |
| THR35 | NaN | 0.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E34HA | 1.00 |
| E34HB2 | 1.00 |
| E34HG2 | 1.00 |
| E34HG3 | 1.00 |
| E34H | 1.00 |
| E34HE2 | 1.00 |
| E34HB3 | 1.00 |
| T35H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU34 | HA | 1.00 | 0.008 | 1.00 | 1.32 |
| GLU34 | HB2 | 1.00 | 0.002 | 1.00 | 9.85 |
| GLU34 | HB3 | 1.00 | 0.002 | 1.00 | 9.85 |
| GLU34 | HG2 | 1.00 | 0.103 | 0.00 | 0.00 |
| GLU34 | HG3 | 1.00 | 0.103 | 0.00 | 0.00 |
| GLU34 | H | 1.00 | 0.004 | 1.00 | -809996.00 |

3.34.8 Detailed Probabilities of GLU34HG2:

Overall probability: 0.333

Overall confidence: 0.750

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU34 | 0.33 | 0.86 |
| THR35 | 0.00 | 0.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E34HA | 1.00 |
| E34HB2 | 1.00 |
| E34HB3 | 1.00 |
| E34HG3 | 1.00 |
| E34H | 1.00 |
| E34HE2 | 1.00 |
| E34HG2 | 1.00 |
| T35H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU34 | HA | 1.00 | 0.081 | 0.00 | 0.00 |
| GLU34 | HB2 | 1.00 | 0.086 | 0.00 | 0.00 |
| GLU34 | HB3 | 1.00 | 0.086 | 0.00 | 0.00 |
| GLU34 | HG2 | 1.00 | 0.015 | 1.00 | 180.23 |
| GLU34 | HG3 | 1.00 | 0.015 | 1.00 | 180.23 |
| GLU34 | H | 1.00 | 0.085 | 0.00 | 0.00 |

3.34.9 Detailed Probabilities of GLU34HG3:

Overall probability: 0.333

Overall confidence: 0.750

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU34 | 0.33 | 0.86 |
| THR35 | 0.00 | 0.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E34HA | 1.00 |
| E34HB2 | 1.00 |
| E34HB3 | 1.00 |
| E34HG2 | 1.00 |
| E34H | 1.00 |
| E34HE2 | 1.00 |
| E34HG3 | 1.00 |
| T35H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU34 | HA | 1.00 | 0.081 | 0.00 | 0.00 |
| GLU34 | HB2 | 1.00 | 0.086 | 0.00 | 0.00 |
| GLU34 | HB3 | 1.00 | 0.086 | 0.00 | 0.00 |
| GLU34 | HG2 | 1.00 | 0.015 | 1.00 | 180.23 |
| GLU34 | HG3 | 1.00 | 0.015 | 1.00 | 180.23 |
| GLU34 | H | 1.00 | 0.085 | 0.00 | 0.00 |

3.34.10 Detailed Probabilities of GLU34H:

Overall probability: 0.771

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU33 | 0.57 | 1.00 |
| GLU34 | 1.00 | 1.00 |
| THR35 | 0.00 | 0.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L33HA | 1.00 |
| L33HB2 | 1.00 |
| L33HB3 | 1.00 |
| L33HG | 0.98 |
| L33H | 1.00 |
| E34HA | 1.00 |
| E34HB2 | 1.00 |
| E34HB3 | 1.00 |
| E34HG2 | 1.00 |
| E34HG3 | 1.00 |
| E34H | 1.00 |
| T35H | 1.00 |

NOESY contacts detailed probability

3.34 *GLU(34)*

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU33 | HA | 1.00 | 0.016 | 1.00 | 0.41 |
| LEU33 | HB2 | 1.00 | 1.433 | 0.00 | 0.00 |
| LEU33 | HB3 | 1.00 | 1.430 | 0.00 | 0.00 |
| LEU33 | HG | 0.98 | 1.433 | 0.02 | 0.00 |
| LEU33 | H | 1.00 | 0.005 | 1.00 | -550022.00 |
| LEU33 | HD11 | 0.51 | 0.000 | 1.00 | 0.06 |
| LEU33 | HD21 | 0.58 | 0.006 | 1.00 | 0.09 |
| GLU34 | HA | 1.00 | 0.009 | 1.00 | 0.64 |
| GLU34 | HB2 | 1.00 | 0.006 | 1.00 | 0.23 |
| GLU34 | HB3 | 1.00 | 0.006 | 1.00 | 0.23 |
| GLU34 | HG2 | 1.00 | 0.008 | 1.00 | 0.25 |
| GLU34 | HG3 | 1.00 | 0.008 | 1.00 | 0.25 |
| GLU34 | H | 1.00 | 0.005 | 1.00 | -2933712.00 |

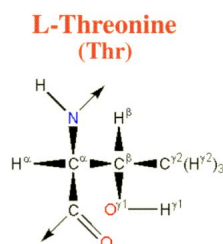
3.35 THR(35)

Figure 25: Image from the BMRB

Residue probability: 0.918

Residue probability confidence: 0.694

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 173.416 | 174.627 | 1.788 | 0.000 | 0.000 |
| CA 3.35.1 | 61.591 | 62.330 | 4.136 | 0.889 | 0.750 |
| CB 3.35.2 | 70.123 | 69.395 | 4.500 | 1.000 | 0.667 |
| CG2 3.35.3 | 21.734 | 21.588 | 1.595 | 0.762 | 0.667 |
| N | NA | – | – | 0.000 | 0.000 |
| HA 3.35.4 | 4.395 | 4.461 | 0.626 | 0.857 | 0.750 |
| HB 3.35.5 | 4.499 | 4.172 | 0.855 | 1.000 | 0.667 |
| HG2 3.35.6 | 1.214 | 1.134 | 0.349 | 1.000 | 0.667 |
| H | NA | – | – | 0.000 | 0.000 |
| HG1 | NA | – | – | 0.000 | 0.000 |

3.35.1 Detailed Probabilities of THR35CA:

Overall probability: 0.889

Overall confidence: 0.750

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU34 | 1.00 | 1.00 |
| THR35 | 1.00 | 0.60 |
| ARG36 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E34HA | 1.00 |
| T35HB | 1.00 |
| T35HG21 | 1.00 |
| T35H | 1.00 |
| T35HG1 | 1.00 |
| T35HA | 1.00 |
| R36H | 1.00 |
| R36HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU34 | HA | 1.00 | 0.017 | 1.00 | 0.16 |
| GLU34 | HB2 | 0.64 | 0.016 | 1.00 | 0.28 |
| GLU34 | HB3 | 0.81 | 0.014 | 1.00 | 0.28 |
| THR35 | HA | 1.00 | 0.002 | 1.00 | 15.29 |
| THR35 | HB | 1.00 | 0.001 | 1.00 | 2.03 |
| THR35 | HG21 | 1.00 | 0.005 | 1.00 | 2.42 |
| ARG36 | HA | 1.00 | 0.056 | 0.00 | 0.00 |
| ARG36 | H | 1.00 | 0.002 | 1.00 | 0.31 |
| ARG36 | HB2 | 0.52 | 0.027 | 1.00 | 0.16 |

3.35.2 Detailed Probabilities of THR35CB:

Overall probability: 1.000

Overall confidence: 0.667

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR35 | 1.00 | 0.60 |
| ARG36 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T35HA | 1.00 |
| T35HG21 | 1.00 |
| T35H | 1.00 |
| T35HG1 | 1.00 |
| T35HB | 1.00 |
| R36H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR35 | HA | 1.00 | 0.006 | 1.00 | 1.43 |
| THR35 | HB | 1.00 | 0.000 | 1.00 | 15.67 |
| THR35 | HG21 | 1.00 | 0.006 | 1.00 | 4.04 |
| ARG36 | H | 1.00 | 0.029 | 1.00 | 0.20 |
| ARG36 | HA | 0.75 | 0.021 | 1.00 | 0.21 |

3.35.3 Detailed Probabilities of THR35CG2:

Overall probability: 0.762

Overall confidence: 0.667

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR35 | 1.00 | 0.60 |
| ARG36 | 0.05 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T35HA | 1.00 |
| T35HB | 1.00 |
| T35HG22 | 1.00 |
| T35H | 1.00 |
| T35HG1 | 1.00 |
| R36H | 0.96 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR35 | HA | 1.00 | 0.020 | 1.00 | 2.96 |
| THR35 | HB | 1.00 | 0.002 | 1.00 | 4.03 |
| THR35 | HG21 | 1.00 | 0.012 | 1.00 | 231.85 |
| ARG36 | H | 0.95 | 0.043 | 0.05 | 0.00 |

3.35.4 Detailed Probabilities of THR35HA:

Overall probability: 0.857

Overall confidence: 0.750

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU34 | 0.00 | 1.00 |
| THR35 | 1.00 | 0.60 |
| ARG36 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E34HA | 1.00 |
| T35HB | 1.00 |
| T35HG21 | 1.00 |
| T35H | 1.00 |
| T35HG1 | 1.00 |
| T35HA | 1.00 |
| R36H | 1.00 |
| R36HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU34 | HA | 1.00 | 0.049 | 0.00 | 0.00 |
| THR35 | HA | 1.00 | 0.002 | 1.00 | 15.29 |
| THR35 | HB | 1.00 | 0.006 | 1.00 | 1.43 |
| THR35 | HG21 | 1.00 | 0.020 | 1.00 | 2.96 |
| ARG36 | HA | 1.00 | 0.017 | 1.00 | 0.60 |
| ARG36 | H | 1.00 | 0.001 | 1.00 | -543497.00 |
| ARG36 | HB2 | 0.52 | 0.014 | 1.00 | 0.09 |

3.35.5 Detailed Probabilities of THR35HB:

Overall probability: 1.000

Overall confidence: 0.667

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR35 | 1.00 | 0.60 |
| ARG36 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T35HA | 1.00 |
| T35HG21 | 1.00 |
| T35H | 1.00 |
| T35HG1 | 1.00 |
| T35HB | 1.00 |
| R36H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR35 | HA | 1.00 | 0.001 | 1.00 | 2.03 |
| THR35 | HB | 1.00 | 0.000 | 1.00 | 15.67 |
| THR35 | HG21 | 1.00 | 0.002 | 1.00 | 4.03 |
| ARG36 | H | 1.00 | 0.004 | 1.00 | -291671.00 |

3.35.6 Detailed Probabilities of THR35HG21:

Overall probability: 1.000

Overall confidence: 0.667

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR35 | 1.00 | 0.60 |
| ARG36 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T35HA | 1.00 |
| T35HB | 1.00 |
| T35HG22 | 1.00 |
| T35H | 1.00 |
| T35HG1 | 1.00 |
| R36H | 0.96 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR35 | HA | 1.00 | 0.005 | 1.00 | 2.42 |
| THR35 | HB | 1.00 | 0.006 | 1.00 | 4.04 |
| THR35 | HG21 | 1.00 | 0.012 | 1.00 | 231.85 |
| ARG36 | H | 0.95 | 0.004 | 1.00 | -194788.00 |

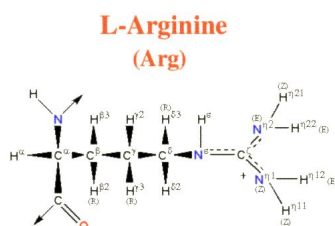


Figure 26: Image from the BMRB

Residue probability: 0.923

Residue probability confidence: 0.835

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 172.402 | 176.453 | 2.303 | 0.000 | 0.000 |
| CA 3.36.1 | 55.068 | 56.803 | 3.326 | 0.980 | 1.000 |
| CB 3.36.2 | 31.942 | 30.892 | 2.424 | 1.000 | 0.889 |
| CG 3.36.3 | 26.200 | 27.247 | 1.538 | 1.000 | 0.778 |
| CD 3.36.4 | 43.472 | 43.189 | 1.415 | 0.861 | 0.667 |
| N 3.36.5 | 117.791 | 120.701 | 3.779 | 1.000 | 0.833 |
| NE | NA | – | – | 0.000 | 0.000 |
| NH1 | NA | – | – | 0.000 | 0.000 |
| NH2 | NA | – | – | 0.000 | 0.000 |
| HA 3.36.6 | 4.735 | 4.301 | 0.495 | 0.729 | 1.000 |
| HB2 3.36.7 | 2.027 | 1.793 | 0.292 | 0.875 | 0.889 |
| HB3 3.36.8 | 1.898 | 1.757 | 0.307 | 0.875 | 0.889 |
| HG2 3.36.9 | 1.622 | 1.559 | 0.294 | 0.975 | 0.800 |
| HG3 3.36.10 | 1.438 | 1.535 | 0.310 | 1.000 | 0.778 |
| HD 3.36.11 | 3.181 | 3.105 | 0.301 | 0.857 | 0.667 |
| H 3.36.12 | 7.318 | 8.248 | 0.623 | 0.920 | 0.833 |
| HE | NA | – | – | 0.000 | 0.000 |
| HH1 | NA | – | – | 0.000 | 0.000 |
| HH2 | NA | – | – | 0.000 | 0.000 |

3.36.1 Detailed Probabilities of ARG36CA:

Overall probability: 0.980

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR35 | 1.00 | 1.00 |
| ARG36 | 0.97 | 1.00 |
| THR37 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T35HA | 1.00 |
| R36HB2 | 1.00 |
| R36HB3 | 1.00 |
| R36HG2 | 1.00 |
| R36HG3 | 1.00 |
| R36HD2 | 0.98 |
| R36H | 1.00 |
| R36HA | 1.00 |
| T37HA | 1.00 |
| T37H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR35 | HA | 1.00 | 0.017 | 1.00 | 0.60 |
| ARG36 | HA | 1.00 | 0.006 | 1.00 | 3.78 |
| ARG36 | HB2 | 1.00 | 0.006 | 1.00 | 1.07 |
| ARG36 | HB3 | 1.00 | 0.009 | 1.00 | 0.69 |
| ARG36 | HG2 | 1.00 | 0.032 | 0.80 | 0.00 |
| ARG36 | HG3 | 1.00 | 0.011 | 1.00 | 0.15 |
| ARG36 | HD2 | 0.98 | 0.010 | 1.00 | 0.55 |
| ARG36 | H | 1.00 | 0.020 | 1.00 | 0.97 |
| THR37 | HA | 1.00 | 0.012 | 1.00 | 0.75 |
| THR37 | H | 1.00 | 0.016 | 1.00 | 0.69 |

3.36.2 Detailed Probabilities of ARG36CB:

Overall probability: 1.000

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG36 | 1.00 | 0.88 |
| THR37 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R36HA | 1.00 |
| R36HB3 | 1.00 |
| R36HG2 | 1.00 |
| R36HG3 | 1.00 |
| R36HD2 | 1.00 |
| R36H | 1.00 |
| R36HE | 1.00 |
| R36HB2 | 1.00 |
| T37H | 1.00 |

NOESY contacts detailed probability

3.36 ARG(36)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG36 | HA | 1.00 | 0.001 | 1.00 | 0.58 |
| ARG36 | HB2 | 1.00 | 0.009 | 1.00 | 17.43 |
| ARG36 | HB3 | 1.00 | 0.005 | 1.00 | 2.83 |
| ARG36 | HG2 | 1.00 | 0.005 | 1.00 | 0.52 |
| ARG36 | HG3 | 1.00 | 0.005 | 1.00 | 0.41 |
| ARG36 | HD2 | 1.00 | 0.011 | 1.00 | 0.53 |
| ARG36 | H | 1.00 | 0.009 | 1.00 | 0.09 |
| THR37 | H | 1.00 | 0.001 | 1.00 | 0.60 |

3.36.3 Detailed Probabilities of ARG36CG:

Overall probability: 1.000

Overall confidence: 0.778

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG36 | 1.00 | 0.78 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R36HA | 1.00 |
| R36HB2 | 1.00 |
| R36HB3 | 1.00 |
| R36HG2 | 1.00 |
| R36HD2 | 1.00 |
| R36H | 1.00 |
| R36HE | 1.00 |
| R36HH11 | 1.00 |
| R36HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG36 | HA | 1.00 | 0.012 | 1.00 | 0.23 |
| ARG36 | HB2 | 1.00 | 0.003 | 1.00 | 0.49 |
| ARG36 | HB3 | 1.00 | 0.000 | 1.00 | 0.60 |
| ARG36 | HG2 | 1.00 | 0.001 | 1.00 | 4.18 |
| ARG36 | HG3 | 1.00 | 0.005 | 1.00 | 7.29 |
| ARG36 | HD2 | 1.00 | 0.010 | 1.00 | 0.90 |
| ARG36 | H | 1.00 | 0.001 | 1.00 | 0.17 |

3.36.4 Detailed Probabilities of ARG36CD:

Overall probability: 0.861

Overall confidence: 0.667

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG36 | 0.86 | 0.67 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R36HA | 0.98 |
| R36HB2 | 1.00 |
| R36HB3 | 1.00 |
| R36HG2 | 1.00 |
| R36HG3 | 1.00 |
| R36HD3 | 1.00 |
| R36HE | 1.00 |
| R36HH11 | 1.00 |
| R36HH21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG36 | HA | 0.97 | 0.056 | 0.03 | 0.00 |
| ARG36 | HB2 | 1.00 | 0.008 | 1.00 | 1.32 |
| ARG36 | HB3 | 1.00 | 0.030 | 1.00 | 0.00 |
| ARG36 | HG2 | 1.00 | 0.001 | 1.00 | 1.23 |
| ARG36 | HG3 | 1.00 | 0.004 | 1.00 | 1.24 |
| ARG36 | HD2 | 1.00 | 0.013 | 1.00 | 52.97 |
| ARG36 | H | 0.86 | 0.001 | 1.00 | 0.12 |

3.36.5 Detailed Probabilities of ARG36N:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR35 | 1.00 | 0.60 |
| ARG36 | 1.00 | 1.00 |
| THR37 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T35HA | 1.00 |
| T35HG22 | 0.95 |
| T35HG1 | 0.97 |
| T35H | 1.00 |
| T35HB | 1.00 |
| R36HA | 1.00 |
| R36HB2 | 1.00 |
| R36HB3 | 1.00 |
| R36HG2 | 1.00 |
| R36HG3 | 1.00 |
| R36H | 1.00 |
| T37H | 1.00 |

NOESY contacts detailed probability

3.36 ARG(36)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR35 | HA | 1.00 | 0.001 | 1.00 | -543497.00 |
| THR35 | HB | 1.00 | 0.004 | 1.00 | -291671.00 |
| THR35 | HG21 | 0.96 | 0.004 | 1.00 | -194788.00 |
| ARG36 | HA | 1.00 | 0.021 | 1.00 | -907678.00 |
| ARG36 | HB2 | 1.00 | 0.000 | 1.00 | -324293.00 |
| ARG36 | HB3 | 1.00 | 0.004 | 1.00 | -542636.00 |
| ARG36 | HG2 | 1.00 | 0.002 | 1.00 | -839150.00 |
| ARG36 | HG3 | 1.00 | 0.003 | 1.00 | -362180.00 |
| ARG36 | H | 1.00 | 0.003 | 1.00 | -7053914.00 |
| ARG36 | HD2 | 0.87 | 0.018 | 1.00 | -138942.00 |
| THR37 | H | 1.00 | 0.001 | 1.00 | -340471.00 |

3.36.6 Detailed Probabilities of ARG36HA:

Overall probability: 0.729

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR35 | 0.50 | 1.00 |
| ARG36 | 0.72 | 1.00 |
| THR37 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T35HA | 1.00 |
| R36HB2 | 1.00 |
| R36HB3 | 1.00 |
| R36HG2 | 1.00 |
| R36HG3 | 1.00 |
| R36HD2 | 0.98 |
| R36H | 1.00 |
| R36HA | 1.00 |
| T37HA | 1.00 |
| T37H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR35 | HA | 1.00 | 0.056 | 0.00 | 0.00 |
| THR35 | HB | 0.75 | 0.021 | 1.00 | 0.21 |
| ARG36 | HA | 1.00 | 0.006 | 1.00 | 3.78 |
| ARG36 | HB2 | 1.00 | 0.001 | 1.00 | 0.58 |
| ARG36 | HB3 | 1.00 | 0.235 | 0.00 | 0.00 |
| ARG36 | HG2 | 1.00 | 0.011 | 1.00 | 0.28 |
| ARG36 | HG3 | 1.00 | 0.012 | 1.00 | 0.23 |
| ARG36 | HD2 | 0.98 | 0.056 | 0.02 | 0.00 |
| ARG36 | H | 1.00 | 0.021 | 1.00 | -907678.00 |
| THR37 | HA | 1.00 | 0.019 | 1.00 | 0.25 |
| THR37 | H | 1.00 | 0.002 | 1.00 | -1981832.00 |

3.36.7 Detailed Probabilities of ARG36HB2:

Overall probability: 0.875

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG36 | 0.86 | 0.88 |
| THR37 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R36HA | 1.00 |
| R36HB3 | 1.00 |
| R36HG2 | 1.00 |
| R36HG3 | 1.00 |
| R36HD2 | 1.00 |
| R36H | 1.00 |
| R36HE | 1.00 |
| R36HB2 | 1.00 |
| T37H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG36 | HA | 1.00 | 0.006 | 1.00 | 1.07 |
| ARG36 | HB2 | 1.00 | 0.009 | 1.00 | 17.43 |
| ARG36 | HB3 | 1.00 | 0.299 | 0.00 | 0.00 |
| ARG36 | HG2 | 1.00 | 0.002 | 1.00 | 0.58 |
| ARG36 | HG3 | 1.00 | 0.003 | 1.00 | 0.49 |
| ARG36 | HD2 | 1.00 | 0.008 | 1.00 | 1.32 |
| ARG36 | H | 1.00 | 0.000 | 1.00 | -324293.00 |
| THR37 | H | 1.00 | 0.005 | 1.00 | -1247812.00 |

3.36.8 Detailed Probabilities of ARG36HB3:

Overall probability: 0.875

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG36 | 0.86 | 0.88 |
| THR37 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R36HA | 1.00 |
| R36HB2 | 1.00 |
| R36HG2 | 1.00 |
| R36HG3 | 1.00 |
| R36HD2 | 1.00 |
| R36H | 1.00 |
| R36HE | 1.00 |
| R36HB3 | 1.00 |
| T37H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG36 | HA | 1.00 | 0.009 | 1.00 | 0.69 |
| ARG36 | HB2 | 1.00 | 0.005 | 1.00 | 2.83 |
| ARG36 | HB3 | 1.00 | 0.428 | 0.00 | 0.00 |
| ARG36 | HG2 | 1.00 | 0.003 | 1.00 | 0.54 |
| ARG36 | HG3 | 1.00 | 0.000 | 1.00 | 0.60 |
| ARG36 | HD2 | 1.00 | 0.030 | 1.00 | 0.00 |
| ARG36 | H | 1.00 | 0.004 | 1.00 | -542636.00 |
| THR37 | H | 1.00 | 0.002 | 1.00 | -1861930.00 |

3.36.9 Detailed Probabilities of ARG36HG2:

Overall probability: 0.975

Overall confidence: 0.800

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG36 | 0.97 | 0.78 |
| THR37 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R36HA | 1.00 |
| R36HB2 | 1.00 |
| R36HB3 | 1.00 |
| R36HG3 | 1.00 |
| R36HD2 | 1.00 |
| R36H | 1.00 |
| R36HE | 1.00 |
| R36HH11 | 1.00 |
| R36HG2 | 1.00 |
| T37H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG36 | HA | 1.00 | 0.032 | 0.80 | 0.00 |
| ARG36 | HB2 | 1.00 | 0.005 | 1.00 | 0.52 |
| ARG36 | HB3 | 1.00 | 0.008 | 1.00 | 0.62 |
| ARG36 | HG2 | 1.00 | 0.001 | 1.00 | 7.71 |
| ARG36 | HG3 | 1.00 | 0.001 | 1.00 | 4.18 |
| ARG36 | HD2 | 1.00 | 0.001 | 1.00 | 1.23 |
| ARG36 | H | 1.00 | 0.002 | 1.00 | -839150.00 |
| THR37 | H | 0.97 | 0.004 | 1.00 | -365003.00 |

3.36.10 Detailed Probabilities of ARG36HG3:

Overall probability: 1.000

Overall confidence: 0.778

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG36 | 1.00 | 0.78 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R36HA | 1.00 |
| R36HB2 | 1.00 |
| R36HB3 | 1.00 |
| R36HG2 | 1.00 |
| R36HD2 | 1.00 |
| R36H | 1.00 |
| R36HE | 1.00 |
| R36HH11 | 1.00 |
| R36HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG36 | HA | 1.00 | 0.011 | 1.00 | 0.15 |
| ARG36 | HB2 | 1.00 | 0.005 | 1.00 | 0.41 |
| ARG36 | HB3 | 1.00 | 0.007 | 1.00 | 0.54 |
| ARG36 | HG2 | 1.00 | 0.005 | 1.00 | 4.21 |
| ARG36 | HG3 | 1.00 | 0.005 | 1.00 | 7.29 |
| ARG36 | HD2 | 1.00 | 0.004 | 1.00 | 1.24 |
| ARG36 | H | 1.00 | 0.003 | 1.00 | -362180.00 |

3.36.11 Detailed Probabilities of ARG36HD2:

Overall probability: 0.857

Overall confidence: 0.667

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG36 | 0.86 | 0.67 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R36HA | 0.98 |
| R36HB2 | 1.00 |
| R36HB3 | 1.00 |
| R36HG2 | 1.00 |
| R36HG3 | 1.00 |
| R36HD3 | 1.00 |
| R36HE | 1.00 |
| R36HH11 | 1.00 |
| R36HH21 | 1.00 |

NOESY contacts detailed probability

3.36 ARG(36)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG36 | HA | 0.97 | 0.010 | 1.00 | 0.55 |
| ARG36 | HB2 | 1.00 | 0.011 | 1.00 | 0.53 |
| ARG36 | HB3 | 1.00 | 0.011 | 1.00 | 0.48 |
| ARG36 | HG2 | 1.00 | 1.156 | 0.00 | 0.00 |
| ARG36 | HG3 | 1.00 | 0.010 | 1.00 | 0.90 |
| ARG36 | HD2 | 1.00 | 0.013 | 1.00 | 52.97 |
| ARG36 | H | 0.86 | 0.018 | 1.00 | -138942.00 |

3.36.12 Detailed Probabilities of ARG36H:

Overall probability: 0.920

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR35 | 0.68 | 0.60 |
| ARG36 | 1.00 | 1.00 |
| THR37 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T35HA | 1.00 |
| T35HG22 | 0.95 |
| T35HG1 | 0.97 |
| T35H | 1.00 |
| T35HB | 1.00 |
| R36HA | 1.00 |
| R36HB2 | 1.00 |
| R36HB3 | 1.00 |
| R36HG2 | 1.00 |
| R36HG3 | 1.00 |
| R36H | 1.00 |
| T37H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR35 | HA | 1.00 | 0.002 | 1.00 | 0.31 |
| THR35 | HB | 1.00 | 0.029 | 1.00 | 0.20 |
| THR35 | HG21 | 0.96 | 0.043 | 0.04 | 0.00 |
| ARG36 | HA | 1.00 | 0.020 | 1.00 | 0.97 |
| ARG36 | HB2 | 1.00 | 0.009 | 1.00 | 0.09 |
| ARG36 | HB3 | 1.00 | 0.005 | 1.00 | 0.14 |
| ARG36 | HG2 | 1.00 | 0.003 | 1.00 | 0.29 |
| ARG36 | HG3 | 1.00 | 0.001 | 1.00 | 0.17 |
| ARG36 | H | 1.00 | 0.003 | 1.00 | -7053914.00 |
| ARG36 | HD2 | 0.87 | 0.001 | 1.00 | 0.12 |
| THR37 | H | 1.00 | 0.009 | 1.00 | -147877.00 |
| THR37 | HA | 0.91 | 0.002 | 1.00 | 0.37 |

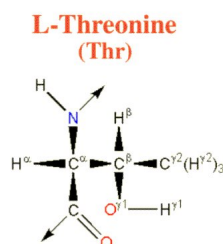
3.37 THR(37)

Figure 27: Image from the BMRB

Residue probability: 0.854

Residue probability confidence: 0.863

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 174.170 | 174.627 | 1.788 | 0.000 | 0.000 |
| CA 3.37.1 | 59.403 | 62.330 | 4.136 | 0.450 | 0.875 |
| CB 3.37.2 | 71.636 | 69.395 | 4.500 | 1.000 | 0.833 |
| CG2 3.37.3 | 21.734 | 21.588 | 1.595 | 1.000 | 0.833 |
| N 3.37.4 | 105.056 | 115.370 | 5.913 | 1.000 | 0.909 |
| HA 3.37.5 | 4.906 | 4.461 | 0.626 | 0.750 | 0.875 |
| HB 3.37.6 | 4.260 | 4.172 | 0.855 | 0.800 | 0.833 |
| HG2 3.37.7 | 1.335 | 1.134 | 0.349 | 1.000 | 0.833 |
| H 3.37.8 | 7.597 | 8.272 | 1.597 | 0.836 | 0.909 |
| HG1 | NA | – | – | 0.000 | 0.000 |

3.37.1 Detailed Probabilities of THR37CA:

Overall probability: 0.450

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG36 | 1.00 | 1.00 |
| THR37 | 0.25 | 0.80 |
| MET38 | 0.30 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R36HA | 1.00 |
| T37HB | 1.00 |
| T37HG21 | 1.00 |
| T37H | 1.00 |
| T37HG1 | 1.00 |
| T37HA | 1.00 |
| M38H | 1.00 |
| M38HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG36 | HA | 1.00 | 0.019 | 1.00 | 0.25 |
| ARG36 | H | 0.91 | 0.002 | 1.00 | 0.37 |
| THR37 | HA | 1.00 | 0.077 | 0.00 | 0.00 |
| THR37 | HB | 1.00 | 0.219 | 0.00 | 0.00 |
| THR37 | HG21 | 1.00 | 0.017 | 1.00 | 0.87 |
| THR37 | H | 1.00 | 0.079 | 0.00 | 0.00 |
| MET38 | HA | 1.00 | 0.144 | 0.00 | 0.00 |
| MET38 | H | 1.00 | 0.034 | 0.60 | 0.00 |

3.37.2 Detailed Probabilities of THR37CB:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR37 | 1.00 | 0.80 |
| MET38 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T37HA | 1.00 |
| T37HG21 | 1.00 |
| T37H | 1.00 |
| T37HG1 | 1.00 |
| T37HB | 1.00 |
| M38H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR37 | HA | 1.00 | 0.006 | 1.00 | 0.85 |
| THR37 | HB | 1.00 | 0.005 | 1.00 | 5.61 |
| THR37 | HG21 | 1.00 | 0.005 | 1.00 | 1.87 |
| THR37 | H | 1.00 | 0.007 | 1.00 | 0.18 |
| MET38 | H | 1.00 | 0.003 | 1.00 | 0.95 |

3.37.3 Detailed Probabilities of THR37CG2:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR37 | 1.00 | 0.80 |
| MET38 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T37HA | 1.00 |
| T37HB | 1.00 |
| T37HG22 | 1.00 |
| T37H | 1.00 |
| T37HG1 | 1.00 |
| M38H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR37 | HA | 1.00 | 0.007 | 1.00 | 0.98 |
| THR37 | HB | 1.00 | 0.005 | 1.00 | 1.76 |
| THR37 | HG21 | 1.00 | 0.005 | 1.00 | 46.74 |
| THR37 | H | 1.00 | 0.004 | 1.00 | 0.59 |
| MET38 | H | 0.97 | 0.004 | 1.00 | 0.45 |
| MET38 | HA | 0.53 | 0.028 | 1.00 | 0.14 |

3.37.4 Detailed Probabilities of THR37N:

Overall probability: 1.000

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG36 | 1.00 | 1.00 |
| THR37 | 1.00 | 0.80 |
| MET38 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R36HB3 | 1.00 |
| R36HG2 | 0.97 |
| R36HA | 1.00 |
| R36H | 1.00 |
| R36HB2 | 1.00 |
| T37HA | 1.00 |
| T37HB | 1.00 |
| T37HG21 | 1.00 |
| T37HG1 | 1.00 |
| T37H | 1.00 |
| M38H | 1.00 |

NOESY contacts detailed probability

3.37 THR(37)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG36 | HA | 1.00 | 0.002 | 1.00 | -1981832.00 |
| ARG36 | HB2 | 1.00 | 0.005 | 1.00 | -1247812.00 |
| ARG36 | HB3 | 1.00 | 0.002 | 1.00 | -1861930.00 |
| ARG36 | HG2 | 0.97 | 0.004 | 1.00 | -365003.00 |
| ARG36 | H | 1.00 | 0.009 | 1.00 | -147877.00 |
| ARG36 | HG3 | 0.94 | 0.005 | 1.00 | -377335.00 |
| ARG36 | HD2 | 0.57 | 0.004 | 1.00 | -229370.00 |
| THR37 | HA | 1.00 | 0.014 | 1.00 | -571267.00 |
| THR37 | HB | 1.00 | 0.007 | 1.00 | -230206.00 |
| THR37 | HG21 | 1.00 | 0.006 | 1.00 | -963064.00 |
| THR37 | H | 1.00 | 0.002 | 1.00 | -11968522.00 |
| MET38 | H | 1.00 | 0.004 | 1.00 | -136577.00 |
| MET38 | HB2 | 0.55 | 0.007 | 1.00 | -365003.00 |

3.37.5 Detailed Probabilities of THR37HA:

Overall probability: 0.750

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG36 | 1.00 | 1.00 |
| THR37 | 0.75 | 0.80 |
| MET38 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R36HA | 1.00 |
| T37HB | 1.00 |
| T37HG21 | 1.00 |
| T37H | 1.00 |
| T37HG1 | 1.00 |
| T37HA | 1.00 |
| M38H | 1.00 |
| M38HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG36 | HA | 1.00 | 0.012 | 1.00 | 0.75 |
| ARG36 | HB3 | 0.82 | 0.019 | 1.00 | 0.11 |
| THR37 | HA | 1.00 | 0.077 | 0.00 | 0.00 |
| THR37 | HB | 1.00 | 0.006 | 1.00 | 0.85 |
| THR37 | HG21 | 1.00 | 0.007 | 1.00 | 0.98 |
| THR37 | H | 1.00 | 0.014 | 1.00 | -571267.00 |
| MET38 | HA | 1.00 | 0.110 | 0.00 | 0.00 |
| MET38 | H | 1.00 | 0.006 | 1.00 | -1650557.00 |

3.37.6 Detailed Probabilities of THR37HB:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR37 | 0.75 | 0.80 |
| MET38 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T37HA | 1.00 |
| T37HG21 | 1.00 |
| T37H | 1.00 |
| T37HG1 | 1.00 |
| T37HB | 1.00 |
| M38H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR37 | HA | 1.00 | 0.219 | 0.00 | 0.00 |
| THR37 | HB | 1.00 | 0.005 | 1.00 | 5.61 |
| THR37 | HG21 | 1.00 | 0.005 | 1.00 | 1.76 |
| THR37 | H | 1.00 | 0.007 | 1.00 | -230206.00 |
| MET38 | H | 1.00 | 0.006 | 1.00 | -1346340.00 |

3.37.7 Detailed Probabilities of THR37HG21:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR37 | 1.00 | 0.80 |
| MET38 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T37HA | 1.00 |
| T37HB | 1.00 |
| T37HG22 | 1.00 |
| T37H | 1.00 |
| T37HG1 | 1.00 |
| M38H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR37 | HA | 1.00 | 0.017 | 1.00 | 0.87 |
| THR37 | HB | 1.00 | 0.005 | 1.00 | 1.87 |
| THR37 | HG21 | 1.00 | 0.005 | 1.00 | 46.74 |
| THR37 | H | 1.00 | 0.006 | 1.00 | -963064.00 |
| MET38 | H | 0.97 | 0.005 | 1.00 | -669420.00 |

3.37.8 Detailed Probabilities of THR37H:

Overall probability: 0.836

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG36 | 0.86 | 1.00 |
| THR37 | 0.75 | 0.80 |
| MET38 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R36HB3 | 1.00 |
| R36HG2 | 0.97 |
| R36HA | 1.00 |
| R36H | 1.00 |
| R36HB2 | 1.00 |
| T37HA | 1.00 |
| T37HB | 1.00 |
| T37HG21 | 1.00 |
| T37HG1 | 1.00 |
| T37H | 1.00 |
| M38H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG36 | HA | 1.00 | 0.016 | 1.00 | 0.69 |
| ARG36 | HB2 | 1.00 | 0.001 | 1.00 | 0.60 |
| ARG36 | HB3 | 1.00 | 0.000 | 1.00 | 0.69 |
| ARG36 | HG2 | 0.97 | 0.282 | 0.03 | 0.00 |
| ARG36 | H | 1.00 | 0.001 | 1.00 | -340471.00 |
| ARG36 | HG3 | 0.94 | 0.002 | 1.00 | 0.19 |
| ARG36 | HD2 | 0.57 | 0.003 | 1.00 | 0.21 |
| THR37 | HA | 1.00 | 0.079 | 0.00 | 0.00 |
| THR37 | HB | 1.00 | 0.007 | 1.00 | 0.18 |
| THR37 | HG21 | 1.00 | 0.004 | 1.00 | 0.59 |
| THR37 | H | 1.00 | 0.002 | 1.00 | -11968522.00 |
| MET38 | H | 1.00 | 0.007 | 1.00 | -160402.00 |

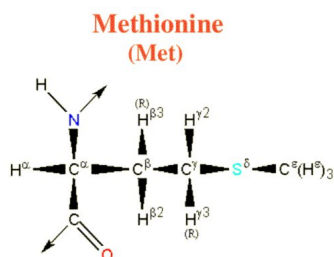
3.38 MET(38)

Figure 28: Image from the BMRB

Residue probability: 0.848

Residue probability confidence: 0.986

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 171.180 | 176.360 | 2.004 | 0.000 | 0.000 |
| CA 3.38.1 | 56.396 | 56.303 | 4.222 | 0.600 | 1.000 |
| CB 3.38.2 | 37.426 | 33.217 | 4.564 | 1.000 | 1.000 |
| CG 3.38.3 | 32.070 | 32.123 | 4.122 | 1.000 | 1.000 |
| CE 3.38.4 | 16.766 | 17.286 | 5.508 | 0.833 | 1.000 |
| N 3.38.5 | 118.861 | 120.023 | 5.158 | 0.909 | 0.917 |
| HA 3.38.6 | 4.185 | 4.409 | 0.504 | 0.583 | 1.000 |
| HB2 3.38.7 | 1.633 | 2.016 | 0.340 | 1.000 | 1.000 |
| HB3 3.38.8 | 1.447 | 1.978 | 0.359 | 0.875 | 1.000 |
| HG2 3.38.9 | 2.108 | 2.410 | 0.360 | 0.750 | 1.000 |
| HG3 3.38.10 | 1.750 | 2.378 | 0.386 | 0.857 | 1.000 |
| HE 3.38.11 | 2.005 | 1.877 | 0.381 | 0.800 | 1.000 |
| H 3.38.12 | 8.376 | 8.269 | 0.585 | 0.969 | 0.917 |

3.38.1 Detailed Probabilities of MET38CA:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR37 | 0.00 | 1.00 |
| MET38 | 0.50 | 1.00 |
| ASP39 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T37HA | 1.00 |
| M38HB2 | 1.00 |
| M38HB3 | 1.00 |
| M38HG2 | 1.00 |
| M38HG3 | 1.00 |
| M38H | 1.00 |
| M38HA | 1.00 |
| D39H | 1.00 |
| D39HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR37 | HA | 1.00 | 0.110 | 0.00 | 0.00 |
| MET38 | HA | 1.00 | 0.158 | 0.00 | 0.00 |
| MET38 | HB2 | 1.00 | 0.005 | 1.00 | 0.67 |
| MET38 | HB3 | 1.00 | 0.003 | 1.00 | 0.44 |
| MET38 | HG2 | 1.00 | 0.141 | 0.00 | 0.00 |
| MET38 | HG3 | 1.00 | 0.122 | 0.00 | 0.00 |
| MET38 | H | 1.00 | 0.022 | 1.00 | 1.42 |
| ASP39 | HA | 1.00 | 0.002 | 1.00 | 0.06 |
| ASP39 | H | 1.00 | 0.002 | 1.00 | 1.42 |
| ASP39 | HB2 | 0.54 | 0.000 | 1.00 | 0.20 |

3.38.2 Detailed Probabilities of MET38CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET38 | 1.00 | 1.00 |
| ASP39 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M38HA | 1.00 |
| M38HB3 | 1.00 |
| M38HG2 | 1.00 |
| M38HG3 | 1.00 |
| M38HE1 | 0.96 |
| M38H | 1.00 |
| M38HB2 | 1.00 |
| D39H | 1.00 |

NOESY contacts detailed probability

3.38 MET(38)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET38 | HA | 1.00 | 0.011 | 1.00 | 0.57 |
| MET38 | HB2 | 1.00 | 0.005 | 1.00 | 4.95 |
| MET38 | HB3 | 1.00 | 0.005 | 1.00 | 2.72 |
| MET38 | HG2 | 1.00 | 0.005 | 1.00 | 0.50 |
| MET38 | HG3 | 1.00 | 0.010 | 1.00 | 1.00 |
| MET38 | HE1 | 0.96 | 0.004 | 1.00 | 0.50 |
| MET38 | H | 1.00 | 0.008 | 1.00 | 0.36 |
| ASP39 | H | 1.00 | 0.016 | 1.00 | 0.36 |

3.38.3 Detailed Probabilities of MET38CG:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET38 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M38HA | 1.00 |
| M38HB2 | 1.00 |
| M38HB3 | 1.00 |
| M38HG2 | 1.00 |
| M38HE1 | 1.00 |
| M38H | 1.00 |
| M38HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET38 | HA | 1.00 | 0.016 | 1.00 | 0.46 |
| MET38 | HB2 | 1.00 | 0.005 | 1.00 | 2.66 |
| MET38 | HB3 | 1.00 | 0.013 | 1.00 | 0.84 |
| MET38 | HG2 | 1.00 | 0.006 | 1.00 | 4.86 |
| MET38 | HG3 | 1.00 | 0.002 | 1.00 | 10.87 |
| MET38 | HE1 | 1.00 | 0.018 | 1.00 | 0.56 |
| MET38 | H | 1.00 | 0.014 | 1.00 | 0.29 |

3.38.4 Detailed Probabilities of MET38CE:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET38 | 0.83 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M38HB2 | 0.96 |
| M38HB3 | 0.97 |
| M38HG2 | 1.00 |
| M38HG3 | 1.00 |
| M38HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET38 | HB2 | 0.96 | 0.006 | 1.00 | 2.63 |
| MET38 | HB3 | 0.97 | 0.006 | 1.00 | 1.61 |
| MET38 | HG2 | 1.00 | 0.100 | 0.00 | 0.00 |
| MET38 | HG3 | 1.00 | 0.011 | 1.00 | 2.06 |
| MET38 | HE1 | 1.00 | 0.003 | 1.00 | 300.68 |
| MET38 | HA | 0.67 | 0.014 | 1.00 | 0.28 |

3.38.5 Detailed Probabilities of MET38N:

Overall probability: 0.909

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR37 | 1.00 | 0.80 |
| MET38 | 0.83 | 1.00 |
| ASP39 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T37HA | 1.00 |
| T37HB | 1.00 |
| T37HG22 | 0.97 |
| T37HG1 | 0.98 |
| T37H | 1.00 |
| M38HA | 1.00 |
| M38HB2 | 1.00 |
| M38HB3 | 1.00 |
| M38HG2 | 1.00 |
| M38HG3 | 1.00 |
| M38H | 1.00 |
| D39H | 1.00 |

NOESY contacts detailed probability

3.38 MET(38)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR37 | HA | 1.00 | 0.006 | 1.00 | -1650557.00 |
| THR37 | HB | 1.00 | 0.006 | 1.00 | -1346340.00 |
| THR37 | HG21 | 0.97 | 0.005 | 1.00 | -669420.00 |
| THR37 | H | 1.00 | 0.007 | 1.00 | -160402.00 |
| MET38 | HA | 1.00 | 0.069 | 0.00 | 0.00 |
| MET38 | HB2 | 1.00 | 0.007 | 1.00 | -656320.00 |
| MET38 | HB3 | 1.00 | 0.006 | 1.00 | -583109.00 |
| MET38 | HG2 | 1.00 | 0.002 | 1.00 | -148073.00 |
| MET38 | HG3 | 1.00 | 0.001 | 1.00 | -150878.00 |
| MET38 | H | 1.00 | 0.003 | 1.00 | -11060844.00 |
| ASP39 | H | 1.00 | 0.021 | 1.00 | -11060844.00 |

3.38.6 Detailed Probabilities of MET38HA:

Overall probability: 0.583

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR37 | 0.50 | 1.00 |
| MET38 | 0.57 | 1.00 |
| ASP39 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T37HA | 1.00 |
| M38HB2 | 1.00 |
| M38HB3 | 1.00 |
| M38HG2 | 1.00 |
| M38HG3 | 1.00 |
| M38H | 1.00 |
| M38HA | 1.00 |
| D39H | 1.00 |
| D39HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR37 | HA | 1.00 | 0.144 | 0.00 | 0.00 |
| THR37 | HG21 | 0.54 | 0.028 | 1.00 | 0.14 |
| MET38 | HA | 1.00 | 0.158 | 0.00 | 0.00 |
| MET38 | HB2 | 1.00 | 0.011 | 1.00 | 0.57 |
| MET38 | HB3 | 1.00 | 0.188 | 0.00 | 0.00 |
| MET38 | HG2 | 1.00 | 0.007 | 1.00 | 0.79 |
| MET38 | HG3 | 1.00 | 0.016 | 1.00 | 0.46 |
| MET38 | H | 1.00 | 0.069 | 0.00 | 0.00 |
| MET38 | HE1 | 0.69 | 0.014 | 1.00 | 0.28 |
| ASP39 | HA | 1.00 | 0.128 | 0.00 | 0.00 |
| ASP39 | H | 1.00 | 0.010 | 1.00 | -2853606.00 |
| ASP39 | HB2 | 0.54 | 0.009 | 1.00 | 0.19 |

3.38.7 Detailed Probabilities of MET38HB2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET38 | 1.00 | 1.00 |
| ASP39 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M38HA | 1.00 |
| M38HB3 | 1.00 |
| M38HG2 | 1.00 |
| M38HG3 | 1.00 |
| M38HE1 | 0.96 |
| M38H | 1.00 |
| M38HB2 | 1.00 |
| D39H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET38 | HA | 1.00 | 0.005 | 1.00 | 0.67 |
| MET38 | HB2 | 1.00 | 0.005 | 1.00 | 4.95 |
| MET38 | HB3 | 1.00 | 0.006 | 1.00 | 3.03 |
| MET38 | HG2 | 1.00 | 0.000 | 1.00 | 1.19 |
| MET38 | HG3 | 1.00 | 0.005 | 1.00 | 2.66 |
| MET38 | HE1 | 0.96 | 0.006 | 1.00 | 2.63 |
| MET38 | H | 1.00 | 0.007 | 1.00 | -656320.00 |
| ASP39 | H | 1.00 | 0.004 | 1.00 | -304383.00 |

3.38.8 Detailed Probabilities of MET38HB3:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET38 | 0.86 | 1.00 |
| ASP39 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M38HA | 1.00 |
| M38HB2 | 1.00 |
| M38HG2 | 1.00 |
| M38HG3 | 1.00 |
| M38HE1 | 0.97 |
| M38H | 1.00 |
| M38HB3 | 1.00 |
| D39H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET38 | HA | 1.00 | 0.003 | 1.00 | 0.44 |
| MET38 | HB2 | 1.00 | 0.005 | 1.00 | 2.72 |
| MET38 | HB3 | 1.00 | 0.178 | 0.00 | 0.00 |
| MET38 | HG2 | 1.00 | 0.004 | 1.00 | 0.58 |
| MET38 | HG3 | 1.00 | 0.013 | 1.00 | 0.84 |
| MET38 | HE1 | 0.97 | 0.006 | 1.00 | 1.61 |
| MET38 | H | 1.00 | 0.006 | 1.00 | -583109.00 |
| ASP39 | H | 1.00 | 0.007 | 1.00 | -306167.00 |

3.38.9 Detailed Probabilities of MET38HG2:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET38 | 0.71 | 1.00 |
| ASP39 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M38HA | 1.00 |
| M38HB2 | 1.00 |
| M38HB3 | 1.00 |
| M38HG3 | 1.00 |
| M38HE1 | 1.00 |
| M38H | 1.00 |
| M38HG2 | 1.00 |
| D39H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET38 | HA | 1.00 | 0.141 | 0.00 | 0.00 |
| MET38 | HB2 | 1.00 | 0.005 | 1.00 | 0.50 |
| MET38 | HB3 | 1.00 | 0.007 | 1.00 | 0.30 |
| MET38 | HG2 | 1.00 | 0.006 | 1.00 | 15.65 |
| MET38 | HG3 | 1.00 | 0.006 | 1.00 | 4.86 |
| MET38 | HE1 | 1.00 | 0.100 | 0.00 | 0.00 |
| MET38 | H | 1.00 | 0.002 | 1.00 | -148073.00 |
| ASP39 | H | 0.97 | 0.004 | 1.00 | -387778.00 |

3.38.10 Detailed Probabilities of MET38HG3:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET38 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M38HA | 1.00 |
| M38HB2 | 1.00 |
| M38HB3 | 1.00 |
| M38HG2 | 1.00 |
| M38HE1 | 1.00 |
| M38H | 1.00 |
| M38HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET38 | HA | 1.00 | 0.122 | 0.00 | 0.00 |
| MET38 | HB2 | 1.00 | 0.010 | 1.00 | 1.00 |
| MET38 | HB3 | 1.00 | 0.008 | 1.00 | 0.76 |
| MET38 | HG2 | 1.00 | 0.003 | 1.00 | 5.60 |
| MET38 | HG3 | 1.00 | 0.002 | 1.00 | 10.87 |
| MET38 | HE1 | 1.00 | 0.011 | 1.00 | 2.06 |
| MET38 | H | 1.00 | 0.001 | 1.00 | -150878.00 |

3.38.11 Detailed Probabilities of MET38HE1:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET38 | 0.80 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M38HB2 | 0.96 |
| M38HB3 | 0.97 |
| M38HG2 | 1.00 |
| M38HG3 | 1.00 |
| M38HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET38 | HB2 | 0.96 | 0.004 | 1.00 | 0.50 |
| MET38 | HB3 | 0.97 | 0.010 | 1.00 | 0.42 |
| MET38 | HG2 | 1.00 | 0.097 | 0.00 | 0.00 |
| MET38 | HG3 | 1.00 | 0.018 | 1.00 | 0.56 |
| MET38 | HE1 | 1.00 | 0.003 | 1.00 | 300.68 |

3.38.12 Detailed Probabilities of MET38H:

Overall probability: 0.969

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR37 | 0.90 | 0.80 |
| MET38 | 1.00 | 1.00 |
| ASP39 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T37HA | 1.00 |
| T37HB | 1.00 |
| T37HG22 | 0.97 |
| T37HG1 | 0.98 |
| T37H | 1.00 |
| M38HA | 1.00 |
| M38HB2 | 1.00 |
| M38HB3 | 1.00 |
| M38HG2 | 1.00 |
| M38HG3 | 1.00 |
| M38H | 1.00 |
| D39H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR37 | HA | 1.00 | 0.034 | 0.60 | 0.00 |
| THR37 | HB | 1.00 | 0.003 | 1.00 | 0.95 |
| THR37 | HG21 | 0.97 | 0.004 | 1.00 | 0.45 |
| THR37 | H | 1.00 | 0.004 | 1.00 | -136577.00 |
| MET38 | HA | 1.00 | 0.022 | 1.00 | 1.42 |
| MET38 | HB2 | 1.00 | 0.008 | 1.00 | 0.36 |
| MET38 | HB3 | 1.00 | 0.009 | 1.00 | 0.36 |
| MET38 | HG2 | 1.00 | 0.016 | 1.00 | 0.35 |
| MET38 | HG3 | 1.00 | 0.014 | 1.00 | 0.29 |
| MET38 | H | 1.00 | 0.003 | 1.00 | -11060844.00 |
| ASP39 | H | 1.00 | 0.021 | 1.00 | -6392216.00 |
| ASP39 | HA | 0.85 | 0.005 | 1.00 | 0.22 |
| ASP39 | HB2 | 0.56 | 0.022 | 1.00 | 0.82 |

3.39 ASP(39)

Figure 29: Image from the BMRB

Residue probability: 0.982

Residue probability confidence: 0.893

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 174.482 | 176.463 | 2.348 | 0.000 | 0.000 |
| CA 3.39.1 | 53.051 | 54.786 | 4.266 | 0.875 | 0.875 |
| CB 3.39.2 | 44.007 | 40.949 | 3.070 | 1.000 | 0.833 |
| N 3.39.3 | 124.613 | 120.550 | 5.690 | 1.000 | 1.000 |
| HD2 | NA | – | – | 0.000 | 0.000 |
| HA 3.39.4 | 5.042 | 4.587 | 0.329 | 1.000 | 0.875 |
| HB2 3.39.5 | 2.563 | 2.708 | 0.282 | 1.000 | 0.833 |
| HB3 3.39.6 | 2.566 | 2.654 | 0.285 | 1.000 | 0.833 |
| H 3.39.7 | 8.400 | 8.304 | 1.027 | 1.000 | 1.000 |

3.39.1 Detailed Probabilities of ASP39CA:

Overall probability: 0.875

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET38 | 0.50 | 1.00 |
| ASP39 | 1.00 | 0.80 |
| PHE40 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M38HA | 1.00 |
| D39HD2 | 1.00 |
| D39HB2 | 1.00 |
| D39HB3 | 1.00 |
| D39H | 1.00 |
| D39HA | 1.00 |
| F40HA | 1.00 |
| F40H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET38 | HA | 1.00 | 0.128 | 0.00 | 0.00 |
| MET38 | H | 0.85 | 0.005 | 1.00 | 0.22 |
| ASP39 | HA | 1.00 | 0.006 | 1.00 | 3.14 |
| ASP39 | HB2 | 1.00 | 0.008 | 1.00 | 0.69 |
| ASP39 | HB3 | 1.00 | 0.005 | 1.00 | 0.69 |
| ASP39 | H | 1.00 | 0.019 | 1.00 | 0.22 |
| PHE40 | HA | 1.00 | 0.024 | 1.00 | 0.26 |
| PHE40 | H | 1.00 | 0.005 | 1.00 | 1.25 |

3.39.2 Detailed Probabilities of ASP39CB:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP39 | 1.00 | 0.80 |
| PHE40 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D39HD2 | 1.00 |
| D39HA | 1.00 |
| D39HB3 | 1.00 |
| D39H | 1.00 |
| D39HB2 | 1.00 |
| F40H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP39 | HA | 1.00 | 0.005 | 1.00 | 0.68 |
| ASP39 | HB2 | 1.00 | 0.001 | 1.00 | 10.93 |
| ASP39 | HB3 | 1.00 | 0.002 | 1.00 | 10.93 |
| ASP39 | H | 1.00 | 0.002 | 1.00 | 0.82 |
| PHE40 | H | 1.00 | 0.002 | 1.00 | 0.20 |
| PHE40 | HA | 0.51 | 0.000 | 1.00 | 0.07 |

3.39.3 Detailed Probabilities of ASP39N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET38 | 1.00 | 1.00 |
| ASP39 | 1.00 | 1.00 |
| PHE40 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M38H | 1.00 |
| M38HG2 | 0.97 |
| M38HB3 | 1.00 |
| M38HB2 | 1.00 |
| M38HA | 1.00 |
| D39HA | 1.00 |
| D39HB2 | 1.00 |
| D39HB3 | 1.00 |
| D39H | 1.00 |
| F40H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET38 | HA | 1.00 | 0.010 | 1.00 | -2853606.00 |
| MET38 | HB2 | 1.00 | 0.004 | 1.00 | -304383.00 |
| MET38 | HB3 | 1.00 | 0.007 | 1.00 | -306167.00 |
| MET38 | HG2 | 0.97 | 0.004 | 1.00 | -387778.00 |
| MET38 | H | 1.00 | 0.021 | 1.00 | -6392216.00 |
| MET38 | HG3 | 0.95 | 0.004 | 1.00 | -291934.00 |
| ASP39 | HA | 1.00 | 0.004 | 1.00 | -403882.00 |
| ASP39 | HB2 | 1.00 | 0.001 | 1.00 | -1661584.00 |
| ASP39 | HB3 | 1.00 | 0.004 | 1.00 | -1661584.00 |
| ASP39 | H | 1.00 | 0.003 | 1.00 | -6392216.00 |
| PHE40 | H | 1.00 | 0.002 | 1.00 | -80896.00 |

3.39.4 Detailed Probabilities of ASP39HA:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET38 | 1.00 | 1.00 |
| ASP39 | 1.00 | 0.80 |
| PHE40 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M38HA | 1.00 |
| D39HD2 | 1.00 |
| D39HB2 | 1.00 |
| D39HB3 | 1.00 |
| D39H | 1.00 |
| D39HA | 1.00 |
| F40HA | 1.00 |
| F40H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET38 | HA | 1.00 | 0.002 | 1.00 | 0.06 |
| ASP39 | HA | 1.00 | 0.006 | 1.00 | 3.14 |
| ASP39 | HB2 | 1.00 | 0.005 | 1.00 | 0.68 |
| ASP39 | HB3 | 1.00 | 0.005 | 1.00 | 0.68 |
| ASP39 | H | 1.00 | 0.004 | 1.00 | -403882.00 |
| PHE40 | HA | 1.00 | 0.024 | 1.00 | 0.31 |
| PHE40 | H | 1.00 | 0.009 | 1.00 | -2265789.00 |

3.39.5 Detailed Probabilities of ASP39HB2:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP39 | 1.00 | 0.80 |
| PHE40 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D39HD2 | 1.00 |
| D39HA | 1.00 |
| D39HB3 | 1.00 |
| D39H | 1.00 |
| D39HB2 | 1.00 |
| F40H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP39 | HA | 1.00 | 0.008 | 1.00 | 0.69 |
| ASP39 | HB2 | 1.00 | 0.001 | 1.00 | 10.93 |
| ASP39 | HB3 | 1.00 | 0.001 | 1.00 | 10.93 |
| ASP39 | H | 1.00 | 0.001 | 1.00 | -1661584.00 |
| PHE40 | H | 1.00 | 0.000 | 1.00 | -534889.00 |
| PHE40 | HA | 0.51 | 0.010 | 1.00 | 0.45 |

3.39.6 Detailed Probabilities of ASP39HB3:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP39 | 1.00 | 0.80 |
| PHE40 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D39HD2 | 1.00 |
| D39HA | 1.00 |
| D39HB2 | 1.00 |
| D39H | 1.00 |
| D39HB3 | 1.00 |
| F40H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP39 | HA | 1.00 | 0.005 | 1.00 | 0.69 |
| ASP39 | HB2 | 1.00 | 0.002 | 1.00 | 10.93 |
| ASP39 | HB3 | 1.00 | 0.002 | 1.00 | 10.93 |
| ASP39 | H | 1.00 | 0.004 | 1.00 | -1661584.00 |
| PHE40 | H | 1.00 | 0.003 | 1.00 | -534889.00 |
| PHE40 | HA | 0.83 | 0.013 | 1.00 | 0.45 |

3.39.7 Detailed Probabilities of ASP39H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET38 | 1.00 | 1.00 |
| ASP39 | 1.00 | 1.00 |
| PHE40 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M38H | 1.00 |
| M38HG2 | 0.97 |
| M38HB3 | 1.00 |
| M38HB2 | 1.00 |
| M38HA | 1.00 |
| D39HA | 1.00 |
| D39HB2 | 1.00 |
| D39HB3 | 1.00 |
| D39H | 1.00 |
| F40H | 1.00 |

NOESY contacts detailed probability

3.39 ASP(39)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET38 | HA | 1.00 | 0.002 | 1.00 | 1.42 |
| MET38 | HB2 | 1.00 | 0.016 | 1.00 | 0.36 |
| MET38 | HB3 | 1.00 | 0.015 | 1.00 | 0.36 |
| MET38 | HG2 | 0.97 | 0.008 | 1.00 | 0.35 |
| MET38 | H | 1.00 | 0.021 | 1.00 | -11060844.00 |
| MET38 | HG3 | 0.95 | 0.010 | 1.00 | 0.29 |
| ASP39 | HA | 1.00 | 0.019 | 1.00 | 0.22 |
| ASP39 | HB2 | 1.00 | 0.002 | 1.00 | 0.82 |
| ASP39 | HB3 | 1.00 | 0.002 | 1.00 | 0.82 |
| ASP39 | H | 1.00 | 0.003 | 1.00 | -6392216.00 |
| PHE40 | H | 1.00 | 0.001 | 1.00 | -156418.00 |

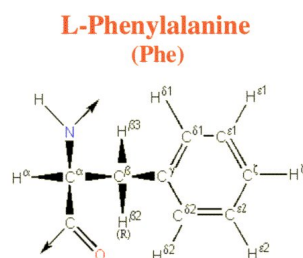
3.40 PHE(40)

Figure 30: Image from the BMRB

Residue probability: 0.829

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | NA | – | – | 0.000 | 0.000 |
| CA 3.40.1 | 53.605 | 58.245 | 3.808 | 0.583 | 1.000 |
| CB 3.40.2 | 38.650 | 40.078 | 3.616 | 0.902 | 1.000 |
| CD1 3.40.3 | 131.700 | 131.234 | 9.579 | 0.889 | 1.000 |
| CD2 3.40.4 | 131.792 | 131.352 | 9.581 | 0.889 | 1.000 |
| CE1 3.40.5 | 130.137 | 130.599 | 3.219 | 1.000 | 1.000 |
| CE2 3.40.6 | 130.304 | 130.633 | 2.839 | 0.857 | 1.000 |
| CZ 3.40.7 | 128.949 | 129.042 | 3.448 | 0.600 | 1.000 |
| N 3.40.8 | 120.948 | 120.315 | 4.931 | 1.000 | 1.000 |
| HA 3.40.9 | 4.913 | 4.625 | 1.237 | 0.929 | 1.000 |
| HB2 3.40.10 | 3.518 | 2.980 | 0.399 | 0.561 | 1.000 |
| HB3 3.40.11 | 2.670 | 2.916 | 0.434 | 0.800 | 1.000 |
| HD1 3.40.12 | 6.671 | 7.037 | 0.347 | 0.778 | 1.000 |
| HD2 3.40.13 | 6.671 | 7.022 | 0.417 | 0.778 | 1.000 |
| HE1 3.40.14 | 6.172 | 7.046 | 0.417 | 1.000 | 1.000 |
| HE2 3.40.15 | 6.172 | 7.043 | 0.400 | 1.000 | 1.000 |
| HZ 3.40.16 | 6.750 | 6.984 | 1.598 | 0.600 | 1.000 |
| H 3.40.17 | 8.836 | 8.375 | 0.710 | 0.923 | 1.000 |

3.40.1 Detailed Probabilities of PHE40CA:

Overall probability: 0.583

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP39 | 1.00 | 1.00 |
| PHE40 | 0.17 | 1.00 |
| PRO41 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D39HA | 1.00 |
| F40HB2 | 1.00 |
| F40HB3 | 1.00 |
| F40HD1 | 1.00 |
| F40HD2 | 1.00 |
| F40H | 1.00 |
| F40HA | 1.00 |
| P41HD2 | 1.00 |
| P41HA | 1.00 |
| P41HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP39 | HA | 1.00 | 0.024 | 1.00 | 0.31 |
| ASP39 | HB2 | 0.51 | 0.010 | 1.00 | 0.45 |
| ASP39 | HB3 | 0.83 | 0.013 | 1.00 | 0.45 |
| PHE40 | HA | 1.00 | 0.025 | 1.00 | 4.15 |
| PHE40 | HB2 | 1.00 | 0.088 | 0.00 | 0.00 |
| PHE40 | HB3 | 1.00 | 0.117 | 0.00 | 0.00 |
| PHE40 | HD1 | 1.00 | 0.040 | 0.00 | 0.00 |
| PHE40 | HD2 | 1.00 | 0.040 | 0.00 | 0.00 |
| PHE40 | H | 1.00 | 0.199 | 0.00 | 0.00 |
| PRO41 | HA | 1.00 | 0.024 | 1.00 | 0.72 |
| PRO41 | HD2 | 1.00 | 0.017 | 1.00 | 0.98 |
| PRO41 | HD3 | 1.00 | 0.005 | 1.00 | 0.99 |

3.40.2 Detailed Probabilities of PHE40CB:

Overall probability: 0.902

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE40 | 1.00 | 1.00 |
| PRO41 | 0.51 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F40HA | 1.00 |
| F40HB3 | 1.00 |
| F40HD1 | 1.00 |
| F40HD2 | 1.00 |
| F40HE2 | 1.00 |
| F40H | 1.00 |
| F40HB2 | 1.00 |
| P41HD3 | 0.98 |
| P41HD2 | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE40 | HA | 1.00 | 0.008 | 1.00 | 0.21 |
| PHE40 | HB2 | 1.00 | 0.000 | 1.00 | 0.94 |
| PHE40 | HB3 | 1.00 | 0.003 | 1.00 | 1.07 |
| PHE40 | HD1 | 1.00 | 0.003 | 1.00 | 0.42 |
| PHE40 | HD2 | 1.00 | 0.003 | 1.00 | 0.42 |
| PHE40 | HE2 | 1.00 | 0.006 | 1.00 | 0.06 |
| PHE40 | H | 1.00 | 0.005 | 1.00 | 0.17 |
| PHE40 | HE1 | 0.90 | 0.006 | 1.00 | 0.06 |
| PRO41 | HD2 | 0.97 | 0.012 | 1.00 | 0.06 |
| PRO41 | HD3 | 0.98 | 0.083 | 0.02 | 0.00 |

3.40.3 Detailed Probabilities of PHE40CD1:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE40 | 0.89 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F40HA | 1.00 |
| F40HB2 | 1.00 |
| F40HB3 | 1.00 |
| F40HD2 | 1.00 |
| F40HE1 | 1.00 |
| F40HE2 | 1.00 |
| F40HZ | 1.00 |
| F40H | 1.00 |
| F40HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE40 | HA | 1.00 | 0.006 | 1.00 | 0.09 |
| PHE40 | HB2 | 1.00 | 0.003 | 1.00 | 0.16 |
| PHE40 | HB3 | 1.00 | 0.000 | 1.00 | 0.17 |
| PHE40 | HD1 | 1.00 | 0.006 | 1.00 | 2.29 |
| PHE40 | HD2 | 1.00 | 0.006 | 1.00 | 2.29 |
| PHE40 | HE1 | 1.00 | 0.002 | 1.00 | 0.40 |
| PHE40 | HE2 | 1.00 | 0.002 | 1.00 | 0.40 |
| PHE40 | HZ | 1.00 | 0.073 | 0.00 | 0.00 |
| PHE40 | H | 1.00 | 0.005 | 1.00 | 0.09 |

3.40.4 Detailed Probabilities of PHE40CD2:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE40 | 0.89 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F40HA | 1.00 |
| F40HB2 | 1.00 |
| F40HB3 | 1.00 |
| F40HD1 | 1.00 |
| F40HE1 | 1.00 |
| F40HE2 | 1.00 |
| F40HZ | 1.00 |
| F40H | 0.99 |
| F40HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE40 | HA | 1.00 | 0.006 | 1.00 | 0.09 |
| PHE40 | HB2 | 1.00 | 0.003 | 1.00 | 0.16 |
| PHE40 | HB3 | 1.00 | 0.000 | 1.00 | 0.17 |
| PHE40 | HD1 | 1.00 | 0.006 | 1.00 | 2.29 |
| PHE40 | HD2 | 1.00 | 0.006 | 1.00 | 2.29 |
| PHE40 | HE1 | 1.00 | 0.002 | 1.00 | 0.40 |
| PHE40 | HE2 | 1.00 | 0.002 | 1.00 | 0.40 |
| PHE40 | HZ | 1.00 | 0.073 | 0.00 | 0.00 |
| PHE40 | H | 0.99 | 0.005 | 1.00 | 0.09 |

3.40.5 Detailed Probabilities of PHE40CE1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE40 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F40HD1 | 1.00 |
| F40HD2 | 1.00 |
| F40HE2 | 1.00 |
| F40HZ | 1.00 |
| F40HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE40 | HD1 | 1.00 | 0.000 | 1.00 | 0.42 |
| PHE40 | HD2 | 1.00 | 0.000 | 1.00 | 0.42 |
| PHE40 | HE1 | 1.00 | 0.001 | 1.00 | 7.85 |
| PHE40 | HE2 | 1.00 | 0.001 | 1.00 | 7.85 |
| PHE40 | HZ | 1.00 | 0.004 | 1.00 | 1.15 |
| PHE40 | HB3 | 0.89 | 0.001 | 1.00 | 0.15 |

3.40.6 Detailed Probabilities of PHE40CE2:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE40 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F40HB2 | 1.00 |
| F40HB3 | 1.00 |
| F40HD1 | 1.00 |
| F40HD2 | 1.00 |
| F40HE1 | 1.00 |
| F40HZ | 1.00 |
| F40HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE40 | HB2 | 1.00 | 0.215 | 0.00 | 0.00 |
| PHE40 | HB3 | 1.00 | 0.001 | 1.00 | 0.15 |
| PHE40 | HD1 | 1.00 | 0.000 | 1.00 | 0.42 |
| PHE40 | HD2 | 1.00 | 0.000 | 1.00 | 0.42 |
| PHE40 | HE1 | 1.00 | 0.001 | 1.00 | 7.85 |
| PHE40 | HE2 | 1.00 | 0.001 | 1.00 | 7.85 |
| PHE40 | HZ | 1.00 | 0.004 | 1.00 | 1.15 |

3.40.7 Detailed Probabilities of PHE40CZ:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE40 | 0.60 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F40HD1 | 1.00 |
| F40HD2 | 1.00 |
| F40HE1 | 1.00 |
| F40HE2 | 1.00 |
| F40HZ | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE40 | HD1 | 1.00 | 0.051 | 0.00 | 0.00 |
| PHE40 | HD2 | 1.00 | 0.051 | 0.00 | 0.00 |
| PHE40 | HE1 | 1.00 | 0.002 | 1.00 | 0.38 |
| PHE40 | HE2 | 1.00 | 0.002 | 1.00 | 0.38 |
| PHE40 | HZ | 1.00 | 0.010 | 1.00 | 1.76 |

3.40.8 Detailed Probabilities of PHE40N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP39 | 1.00 | 1.00 |
| PHE40 | 1.00 | 1.00 |
| PRO41 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D39HB2 | 1.00 |
| D39HB3 | 1.00 |
| D39H | 1.00 |
| D39HA | 1.00 |
| F40HA | 1.00 |
| F40HB2 | 1.00 |
| F40HB3 | 1.00 |
| F40HD1 | 1.00 |
| F40HD2 | 0.99 |
| F40H | 1.00 |
| P41HD3 | 0.97 |
| P41HD2 | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP39 | HA | 1.00 | 0.009 | 1.00 | -2265789.00 |
| ASP39 | HB2 | 1.00 | 0.000 | 1.00 | -534889.00 |
| ASP39 | HB3 | 1.00 | 0.003 | 1.00 | -534889.00 |
| ASP39 | H | 1.00 | 0.001 | 1.00 | -156418.00 |
| PHE40 | HA | 1.00 | 0.008 | 1.00 | -569242.00 |
| PHE40 | HB2 | 1.00 | 0.000 | 1.00 | -611653.00 |
| PHE40 | HB3 | 1.00 | 0.005 | 1.00 | -437315.00 |
| PHE40 | HD1 | 1.00 | 0.004 | 1.00 | -927565.00 |
| PHE40 | HD2 | 0.99 | 0.004 | 1.00 | -927565.00 |
| PHE40 | H | 1.00 | 0.003 | 1.00 | -8874386.00 |
| PRO41 | HD2 | 0.98 | 0.016 | 1.00 | -193960.00 |
| PRO41 | HD3 | 0.97 | 0.006 | 1.00 | -364200.00 |

3.40.9 Detailed Probabilities of PHE40HA:

Overall probability: 0.929

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP39 | 1.00 | 1.00 |
| PHE40 | 1.00 | 1.00 |
| PRO41 | 0.80 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D39HA | 1.00 |
| F40HB2 | 1.00 |
| F40HB3 | 1.00 |
| F40HD1 | 1.00 |
| F40HD2 | 1.00 |
| F40H | 1.00 |
| F40HA | 1.00 |
| P41HD2 | 1.00 |
| P41HA | 1.00 |
| P41HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP39 | HA | 1.00 | 0.024 | 1.00 | 0.26 |
| ASP39 | HB2 | 0.51 | 0.000 | 1.00 | 0.07 |
| ASP39 | HB3 | 0.83 | 0.000 | 1.00 | 0.07 |
| PHE40 | HA | 1.00 | 0.025 | 1.00 | 4.15 |
| PHE40 | HB2 | 1.00 | 0.008 | 1.00 | 0.21 |
| PHE40 | HB3 | 1.00 | 0.014 | 1.00 | 0.34 |
| PHE40 | HD1 | 1.00 | 0.006 | 1.00 | 0.09 |
| PHE40 | HD2 | 1.00 | 0.006 | 1.00 | 0.09 |
| PHE40 | H | 1.00 | 0.008 | 1.00 | -569242.00 |
| PRO41 | HA | 1.00 | 0.065 | 0.00 | 0.00 |
| PRO41 | HD2 | 1.00 | 0.009 | 1.00 | 0.97 |
| PRO41 | HD3 | 1.00 | 0.010 | 1.00 | 0.81 |
| PRO41 | HB3 | 0.79 | 0.003 | 1.00 | 0.08 |
| PRO41 | HG2 | 0.91 | 0.004 | 1.00 | 0.26 |

3.40.10 Detailed Probabilities of PHE40HB2:

Overall probability: 0.561

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE40 | 0.71 | 1.00 |
| PRO41 | 0.03 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F40HA | 1.00 |
| F40HB3 | 1.00 |
| F40HD1 | 1.00 |
| F40HD2 | 1.00 |
| F40HE2 | 1.00 |
| F40H | 1.00 |
| F40HB2 | 1.00 |
| P41HD3 | 0.98 |
| P41HD2 | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE40 | HA | 1.00 | 0.088 | 0.00 | 0.00 |
| PHE40 | HB2 | 1.00 | 0.000 | 1.00 | 0.94 |
| PHE40 | HB3 | 1.00 | 0.001 | 1.00 | 1.15 |
| PHE40 | HD1 | 1.00 | 0.003 | 1.00 | 0.16 |
| PHE40 | HD2 | 1.00 | 0.003 | 1.00 | 0.16 |
| PHE40 | HE2 | 1.00 | 0.215 | 0.00 | 0.00 |
| PHE40 | H | 1.00 | 0.000 | 1.00 | -611653.00 |
| PRO41 | HD2 | 0.97 | 0.079 | 0.03 | 0.00 |
| PRO41 | HD3 | 0.98 | 0.079 | 0.02 | 0.00 |

3.40.11 Detailed Probabilities of PHE40HB3:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE40 | 0.75 | 1.00 |
| PRO41 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F40HA | 1.00 |
| F40HB2 | 1.00 |
| F40HD1 | 1.00 |
| F40HD2 | 1.00 |
| F40HE2 | 1.00 |
| F40H | 1.00 |
| F40HB3 | 1.00 |
| P41HD2 | 0.98 |
| P41HD3 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE40 | HA | 1.00 | 0.117 | 0.00 | 0.00 |
| PHE40 | HB2 | 1.00 | 0.003 | 1.00 | 1.07 |
| PHE40 | HB3 | 1.00 | 0.849 | 0.00 | 0.00 |
| PHE40 | HD1 | 1.00 | 0.000 | 1.00 | 0.17 |
| PHE40 | HD2 | 1.00 | 0.000 | 1.00 | 0.17 |
| PHE40 | HE2 | 1.00 | 0.001 | 1.00 | 0.15 |
| PHE40 | H | 1.00 | 0.005 | 1.00 | -437315.00 |
| PHE40 | HE1 | 0.89 | 0.001 | 1.00 | 0.15 |
| PRO41 | HD2 | 0.98 | 0.006 | 1.00 | 0.10 |
| PRO41 | HD3 | 0.99 | 0.015 | 1.00 | 0.08 |

3.40.12 Detailed Probabilities of PHE40HD1:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE40 | 0.78 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F40HA | 1.00 |
| F40HB2 | 1.00 |
| F40HB3 | 1.00 |
| F40HD2 | 1.00 |
| F40HE1 | 1.00 |
| F40HE2 | 1.00 |
| F40HZ | 1.00 |
| F40H | 1.00 |
| F40HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE40 | HA | 1.00 | 0.040 | 0.00 | 0.00 |
| PHE40 | HB2 | 1.00 | 0.003 | 1.00 | 0.42 |
| PHE40 | HB3 | 1.00 | 0.004 | 1.00 | 0.56 |
| PHE40 | HD1 | 1.00 | 0.006 | 1.00 | 2.29 |
| PHE40 | HD2 | 1.00 | 0.006 | 1.00 | 2.29 |
| PHE40 | HE1 | 1.00 | 0.000 | 1.00 | 0.42 |
| PHE40 | HE2 | 1.00 | 0.000 | 1.00 | 0.42 |
| PHE40 | HZ | 1.00 | 0.051 | 0.00 | 0.00 |
| PHE40 | H | 1.00 | 0.004 | 1.00 | -927565.00 |

3.40.13 Detailed Probabilities of PHE40HD2:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE40 | 0.78 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F40HA | 1.00 |
| F40HB2 | 1.00 |
| F40HB3 | 1.00 |
| F40HD1 | 1.00 |
| F40HE1 | 1.00 |
| F40HE2 | 1.00 |
| F40HZ | 1.00 |
| F40H | 0.99 |
| F40HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE40 | HA | 1.00 | 0.040 | 0.00 | 0.00 |
| PHE40 | HB2 | 1.00 | 0.003 | 1.00 | 0.42 |
| PHE40 | HB3 | 1.00 | 0.004 | 1.00 | 0.56 |
| PHE40 | HD1 | 1.00 | 0.006 | 1.00 | 2.29 |
| PHE40 | HD2 | 1.00 | 0.006 | 1.00 | 2.29 |
| PHE40 | HE1 | 1.00 | 0.000 | 1.00 | 0.42 |
| PHE40 | HE2 | 1.00 | 0.000 | 1.00 | 0.42 |
| PHE40 | HZ | 1.00 | 0.051 | 0.00 | 0.00 |
| PHE40 | H | 0.99 | 0.004 | 1.00 | -927565.00 |

3.40.14 Detailed Probabilities of PHE40HE1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE40 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F40HD1 | 1.00 |
| F40HD2 | 1.00 |
| F40HE2 | 1.00 |
| F40HZ | 1.00 |
| F40HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE40 | HD1 | 1.00 | 0.002 | 1.00 | 0.40 |
| PHE40 | HD2 | 1.00 | 0.002 | 1.00 | 0.40 |
| PHE40 | HE1 | 1.00 | 0.001 | 1.00 | 7.85 |
| PHE40 | HE2 | 1.00 | 0.001 | 1.00 | 7.85 |
| PHE40 | HZ | 1.00 | 0.002 | 1.00 | 0.38 |
| PHE40 | HB2 | 0.90 | 0.006 | 1.00 | 0.06 |
| PHE40 | HB3 | 0.89 | 0.002 | 1.00 | 0.09 |

3.40.15 Detailed Probabilities of PHE40HE2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE40 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F40HB2 | 1.00 |
| F40HB3 | 1.00 |
| F40HD1 | 1.00 |
| F40HD2 | 1.00 |
| F40HE1 | 1.00 |
| F40HZ | 1.00 |
| F40HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE40 | HB2 | 1.00 | 0.006 | 1.00 | 0.06 |
| PHE40 | HB3 | 1.00 | 0.002 | 1.00 | 0.09 |
| PHE40 | HD1 | 1.00 | 0.002 | 1.00 | 0.40 |
| PHE40 | HD2 | 1.00 | 0.002 | 1.00 | 0.40 |
| PHE40 | HE1 | 1.00 | 0.001 | 1.00 | 7.85 |
| PHE40 | HE2 | 1.00 | 0.001 | 1.00 | 7.85 |
| PHE40 | HZ | 1.00 | 0.002 | 1.00 | 0.38 |

3.40.16 Detailed Probabilities of PHE40HZ:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE40 | 0.60 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F40HD1 | 1.00 |
| F40HD2 | 1.00 |
| F40HE1 | 1.00 |
| F40HE2 | 1.00 |
| F40HZ | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE40 | HD1 | 1.00 | 0.073 | 0.00 | 0.00 |
| PHE40 | HD2 | 1.00 | 0.073 | 0.00 | 0.00 |
| PHE40 | HE1 | 1.00 | 0.004 | 1.00 | 1.15 |
| PHE40 | HE2 | 1.00 | 0.004 | 1.00 | 1.15 |
| PHE40 | HZ | 1.00 | 0.010 | 1.00 | 1.76 |

3.40.17 Detailed Probabilities of PHE40H:

Overall probability: 0.923

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP39 | 1.00 | 1.00 |
| PHE40 | 0.83 | 1.00 |
| PRO41 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D39HB2 | 1.00 |
| D39HB3 | 1.00 |
| D39H | 1.00 |
| D39HA | 1.00 |
| F40HA | 1.00 |
| F40HB2 | 1.00 |
| F40HB3 | 1.00 |
| F40HD1 | 1.00 |
| F40HD2 | 0.99 |
| F40H | 1.00 |
| P41HD3 | 0.97 |
| P41HD2 | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP39 | HA | 1.00 | 0.005 | 1.00 | 1.25 |
| ASP39 | HB2 | 1.00 | 0.002 | 1.00 | 0.20 |
| ASP39 | HB3 | 1.00 | 0.002 | 1.00 | 0.20 |
| ASP39 | H | 1.00 | 0.002 | 1.00 | -80896.00 |
| PHE40 | HA | 1.00 | 0.199 | 0.00 | 0.00 |
| PHE40 | HB2 | 1.00 | 0.005 | 1.00 | 0.17 |
| PHE40 | HB3 | 1.00 | 0.003 | 1.00 | 0.16 |
| PHE40 | HD1 | 1.00 | 0.005 | 1.00 | 0.09 |
| PHE40 | HD2 | 0.99 | 0.005 | 1.00 | 0.09 |
| PHE40 | H | 1.00 | 0.003 | 1.00 | -8874386.00 |
| PRO41 | HD2 | 0.98 | 0.004 | 1.00 | 0.10 |
| PRO41 | HD3 | 0.97 | 0.001 | 1.00 | 0.11 |
| PRO41 | HA | 0.78 | 0.014 | 1.00 | 0.07 |

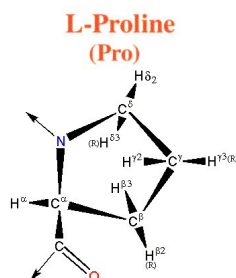
3.41 PRO(41)

Figure 31: Image from the BMRB

Residue probability: 0.879

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 175.938 | 175.173 | 13.901 | 0.000 | 0.000 |
| CA 3.41.1 | 64.334 | 62.931 | 13.301 | 0.720 | 1.000 |
| CB 3.41.2 | 32.589 | 33.632 | 13.629 | 1.000 | 1.000 |
| CG 3.41.3 | 27.140 | 28.412 | 13.801 | 0.817 | 1.000 |
| CD 3.41.4 | 50.490 | 49.797 | 3.175 | 0.903 | 1.000 |
| N | NA | – | – | 0.000 | 0.000 |
| HA 3.41.5 | 4.620 | 4.332 | 0.427 | 0.889 | 1.000 |
| HB2 3.41.6 | 2.486 | 2.099 | 0.501 | 1.000 | 1.000 |
| HB3 3.41.7 | 2.114 | 2.052 | 0.596 | 0.943 | 1.000 |
| HG 3.41.8 | 2.076 | 1.927 | 0.364 | 0.967 | 1.000 |
| HD2 3.41.9 | 3.667 | 3.640 | 0.682 | 0.751 | 1.000 |
| HD3 3.41.10 | 3.435 | 3.558 | 0.522 | 0.803 | 1.000 |

3.41.1 Detailed Probabilities of PRO41CA:

Overall probability: 0.720

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE40 | 0.50 | 1.00 |
| PRO41 | 0.83 | 1.00 |
| THR42 | 0.60 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F40HA | 1.00 |
| P41HB2 | 1.00 |
| P41HB3 | 1.00 |
| P41HG2 | 1.00 |
| P41HD2 | 1.00 |
| P41HD3 | 1.00 |
| P41HA | 1.00 |
| T42HA | 1.00 |
| T42H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE40 | HA | 1.00 | 0.065 | 0.00 | 0.00 |
| PHE40 | H | 0.78 | 0.014 | 1.00 | 0.07 |
| PRO41 | HA | 1.00 | 0.007 | 1.00 | 22.35 |
| PRO41 | HB2 | 1.00 | 0.005 | 1.00 | 4.04 |
| PRO41 | HB3 | 1.00 | 0.008 | 1.00 | 1.94 |
| PRO41 | HG2 | 1.00 | 0.030 | 1.00 | 1.94 |
| PRO41 | HD2 | 1.00 | 0.041 | 0.00 | 0.00 |
| PRO41 | HD3 | 1.00 | 0.004 | 1.00 | 0.31 |
| THR42 | HA | 1.00 | 0.002 | 1.00 | 0.44 |
| THR42 | H | 1.00 | 0.038 | 0.20 | 0.00 |

3.41.2 Detailed Probabilities of PRO41CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO41 | 1.00 | 1.00 |
| THR42 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P41HA | 1.00 |
| P41HB2 | 1.00 |
| P41HG2 | 1.00 |
| P41HD2 | 1.00 |
| P41HD3 | 1.00 |
| P41HB3 | 1.00 |
| T42H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO41 | HA | 1.00 | 0.008 | 1.00 | 1.18 |
| PRO41 | HB2 | 1.00 | 0.008 | 1.00 | 5.52 |
| PRO41 | HB3 | 1.00 | 0.012 | 1.00 | 15.65 |
| PRO41 | HG2 | 1.00 | 0.026 | 1.00 | 15.65 |
| PRO41 | HD2 | 1.00 | 0.005 | 1.00 | 0.33 |
| PRO41 | HD3 | 1.00 | 0.000 | 1.00 | 0.36 |
| THR42 | H | 1.00 | 0.005 | 1.00 | 0.29 |

3.41.3 Detailed Probabilities of PRO41CG:

Overall probability: 0.817

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO41 | 0.82 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P41HA | 1.00 |
| P41HB2 | 1.00 |
| P41HB3 | 1.00 |
| P41HG3 | 1.00 |
| P41HD2 | 1.00 |
| P41HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO41 | HA | 1.00 | 0.005 | 1.00 | 0.60 |
| PRO41 | HB2 | 1.00 | 0.009 | 1.00 | 2.08 |
| PRO41 | HB3 | 1.00 | 0.031 | 0.90 | 0.00 |
| PRO41 | HG2 | 1.00 | 0.007 | 1.00 | 31.34 |
| PRO41 | HD2 | 1.00 | 0.072 | 0.00 | 0.00 |
| PRO41 | HD3 | 1.00 | 0.002 | 1.00 | 1.27 |

3.41.4 Detailed Probabilities of PRO41CD:

Overall probability: 0.903

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE40 | 0.84 | 1.00 |
| PRO41 | 0.97 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F40H | 0.98 |
| F40HB2 | 0.97 |
| F40HA | 1.00 |
| F40HB3 | 0.98 |
| P41HA | 1.00 |
| P41HB2 | 1.00 |
| P41HB3 | 1.00 |
| P41HG2 | 1.00 |
| P41HD3 | 1.00 |
| P41HD2 | 1.00 |

NOESY contacts detailed probability

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE40 | HA | 1.00 | 0.009 | 1.00 | 0.97 |
| PHE40 | HB2 | 0.97 | 0.079 | 0.03 | 0.00 |
| PHE40 | HB3 | 0.98 | 0.006 | 1.00 | 0.10 |
| PHE40 | H | 0.98 | 0.004 | 1.00 | 0.10 |
| PHE40 | HD1 | 0.74 | 0.010 | 1.00 | 0.10 |
| PHE40 | HD2 | 0.55 | 0.010 | 1.00 | 0.10 |
| PRO41 | HA | 1.00 | 0.015 | 1.00 | 0.25 |
| PRO41 | HB2 | 1.00 | 0.008 | 1.00 | 0.24 |
| PRO41 | HB3 | 1.00 | 0.032 | 0.80 | 0.00 |
| PRO41 | HG2 | 1.00 | 0.006 | 1.00 | 1.38 |
| PRO41 | HD2 | 1.00 | 0.010 | 1.00 | 5.13 |
| PRO41 | HD3 | 1.00 | 0.004 | 1.00 | 3.77 |

3.41.5 Detailed Probabilities of PRO41HA:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE40 | 1.00 | 1.00 |
| PRO41 | 1.00 | 1.00 |
| THR42 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F40HA | 1.00 |
| P41HB2 | 1.00 |
| P41HB3 | 1.00 |
| P41HG2 | 1.00 |
| P41HD2 | 1.00 |
| P41HD3 | 1.00 |
| P41HA | 1.00 |
| T42HA | 1.00 |
| T42H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE40 | HA | 1.00 | 0.024 | 1.00 | 0.72 |
| PRO41 | HA | 1.00 | 0.007 | 1.00 | 22.35 |
| PRO41 | HB2 | 1.00 | 0.007 | 1.00 | 2.53 |
| PRO41 | HB3 | 1.00 | 0.008 | 1.00 | 1.18 |
| PRO41 | HG2 | 1.00 | 0.005 | 1.00 | 0.60 |
| PRO41 | HD2 | 1.00 | 0.015 | 1.00 | 0.25 |
| PRO41 | HD3 | 1.00 | 0.019 | 1.00 | 0.22 |
| THR42 | HA | 1.00 | 0.130 | 0.00 | 0.00 |
| THR42 | H | 1.00 | 0.012 | 1.00 | -515210.00 |

3.41.6 Detailed Probabilities of PRO41HB2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO41 | 1.00 | 1.00 |
| THR42 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P41HA | 1.00 |
| P41HB3 | 1.00 |
| P41HG2 | 1.00 |
| P41HD2 | 1.00 |
| P41HD3 | 1.00 |
| P41HB2 | 1.00 |
| T42HA | 0.98 |
| T42H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO41 | HA | 1.00 | 0.005 | 1.00 | 4.04 |
| PRO41 | HB2 | 1.00 | 0.001 | 1.00 | 12.02 |
| PRO41 | HB3 | 1.00 | 0.008 | 1.00 | 5.52 |
| PRO41 | HG2 | 1.00 | 0.009 | 1.00 | 2.08 |
| PRO41 | HD2 | 1.00 | 0.008 | 1.00 | 0.24 |
| PRO41 | HD3 | 1.00 | 0.007 | 1.00 | 0.32 |
| THR42 | HA | 0.98 | 0.012 | 1.00 | 0.06 |
| THR42 | H | 1.00 | 0.011 | 1.00 | -349722.00 |

3.41.7 Detailed Probabilities of PRO41HB3:

Overall probability: 0.943

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO41 | 0.93 | 1.00 |
| THR42 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P41HA | 1.00 |
| P41HB2 | 1.00 |
| P41HG2 | 1.00 |
| P41HD2 | 1.00 |
| P41HD3 | 1.00 |
| P41HB3 | 1.00 |
| T42H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO41 | HA | 1.00 | 0.008 | 1.00 | 1.94 |
| PRO41 | HB2 | 1.00 | 0.006 | 1.00 | 6.93 |
| PRO41 | HB3 | 1.00 | 0.012 | 1.00 | 15.65 |
| PRO41 | HG2 | 1.00 | 0.031 | 0.90 | 0.00 |
| PRO41 | HD2 | 1.00 | 0.032 | 0.80 | 0.00 |
| PRO41 | HD3 | 1.00 | 0.031 | 0.90 | 0.00 |
| THR42 | H | 1.00 | 0.026 | 1.00 | -1809049.00 |

3.41.8 Detailed Probabilities of PRO41HG2:

Overall probability: 0.967

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO41 | 0.97 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P41HA | 1.00 |
| P41HB2 | 1.00 |
| P41HB3 | 1.00 |
| P41HG3 | 1.00 |
| P41HD2 | 1.00 |
| P41HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO41 | HA | 1.00 | 0.030 | 1.00 | 1.94 |
| PRO41 | HB2 | 1.00 | 0.032 | 0.80 | 0.00 |
| PRO41 | HB3 | 1.00 | 0.026 | 1.00 | 15.65 |
| PRO41 | HG2 | 1.00 | 0.007 | 1.00 | 31.34 |
| PRO41 | HD2 | 1.00 | 0.006 | 1.00 | 1.38 |
| PRO41 | HD3 | 1.00 | 0.007 | 1.00 | 1.40 |

3.41.9 Detailed Probabilities of PRO41HD2:

Overall probability: 0.751

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE40 | 0.84 | 1.00 |
| PRO41 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F40H | 0.98 |
| F40HB2 | 0.97 |
| F40HA | 1.00 |
| F40HB3 | 0.98 |
| P41HA | 1.00 |
| P41HB2 | 1.00 |
| P41HB3 | 1.00 |
| P41HG2 | 1.00 |
| P41HD3 | 1.00 |
| P41HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE40 | HA | 1.00 | 0.017 | 1.00 | 0.98 |
| PHE40 | HB2 | 0.97 | 0.012 | 1.00 | 0.06 |
| PHE40 | HB3 | 0.98 | 0.148 | 0.02 | 0.00 |
| PHE40 | H | 0.98 | 0.016 | 1.00 | -193960.00 |
| PHE40 | HD1 | 0.74 | 0.008 | 1.00 | 0.13 |
| PHE40 | HD2 | 0.55 | 0.008 | 1.00 | 0.13 |
| PRO41 | HA | 1.00 | 0.041 | 0.00 | 0.00 |
| PRO41 | HB2 | 1.00 | 0.007 | 1.00 | 0.35 |
| PRO41 | HB3 | 1.00 | 0.005 | 1.00 | 0.33 |
| PRO41 | HG2 | 1.00 | 0.072 | 0.00 | 0.00 |
| PRO41 | HD2 | 1.00 | 0.010 | 1.00 | 5.13 |
| PRO41 | HD3 | 1.00 | 0.010 | 1.00 | 3.70 |

3.41.10 Detailed Probabilities of PRO41HD3:

Overall probability: 0.803

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE40 | 0.51 | 1.00 |
| PRO41 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F40H | 0.97 |
| F40HB2 | 0.98 |
| F40HA | 1.00 |
| F40HB3 | 0.99 |
| P41HA | 1.00 |
| P41HB2 | 1.00 |
| P41HB3 | 1.00 |
| P41HG2 | 1.00 |
| P41HD2 | 1.00 |
| P41HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE40 | HA | 1.00 | 0.005 | 1.00 | 0.99 |
| PHE40 | HB2 | 0.98 | 0.083 | 0.02 | 0.00 |
| PHE40 | HB3 | 0.99 | 0.084 | 0.01 | 0.00 |
| PHE40 | H | 0.97 | 0.006 | 1.00 | -364200.00 |
| PRO41 | HA | 1.00 | 0.004 | 1.00 | 0.31 |
| PRO41 | HB2 | 1.00 | 0.001 | 1.00 | 0.46 |
| PRO41 | HB3 | 1.00 | 0.000 | 1.00 | 0.36 |
| PRO41 | HG2 | 1.00 | 0.002 | 1.00 | 1.27 |
| PRO41 | HD2 | 1.00 | 0.004 | 1.00 | 3.77 |
| PRO41 | HD3 | 1.00 | 0.004 | 1.00 | 5.16 |

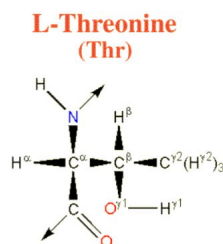
3.42 THR(42)

Figure 32: Image from the BMRB

Residue probability: 0.731

Residue probability confidence: 0.867

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | NA | – | – | 0.000 | 0.000 |
| CA 3.42.1 | 57.417 | 62.330 | 4.136 | 0.732 | 0.909 |
| CB 3.42.2 | 70.881 | 69.395 | 4.500 | 0.430 | 0.857 |
| CG2 3.42.3 | 21.440 | 21.588 | 1.595 | 0.825 | 0.800 |
| N 3.42.4 | 104.189 | 115.370 | 5.913 | 0.909 | 0.900 |
| HA 3.42.5 | 4.980 | 4.461 | 0.626 | 0.833 | 0.909 |
| HB 3.42.6 | 4.489 | 4.172 | 0.855 | 0.779 | 0.857 |
| HG2 3.42.7 | 1.239 | 1.134 | 0.349 | 0.575 | 0.800 |
| H 3.42.8 | 7.123 | 8.272 | 1.597 | 0.768 | 0.900 |
| HG1 | NA | – | – | 0.000 | 0.000 |

3.42.1 Detailed Probabilities of THR42CA:

Overall probability: 0.732

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO41 | 0.50 | 1.00 |
| THR42 | 1.00 | 0.80 |
| PRO43 | 0.61 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P41HB2 | 0.98 |
| P41HA | 1.00 |
| T42HB | 1.00 |
| T42HG21 | 1.00 |
| T42H | 1.00 |
| T42HG1 | 1.00 |
| T42HA | 1.00 |
| P43HD2 | 1.00 |
| P43HD3 | 1.00 |
| P43HG2 | 0.95 |
| P43HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO41 | HA | 1.00 | 0.130 | 0.00 | 0.00 |
| PRO41 | HB2 | 0.98 | 0.012 | 1.00 | 0.06 |
| THR42 | HA | 1.00 | 0.003 | 1.00 | 7.68 |
| THR42 | HB | 1.00 | 0.001 | 1.00 | 1.11 |
| THR42 | HG21 | 1.00 | 0.004 | 1.00 | 1.19 |
| THR42 | H | 1.00 | 0.006 | 1.00 | 0.66 |
| PRO43 | HA | 1.00 | 0.024 | 1.00 | 0.18 |
| PRO43 | HG2 | 0.95 | 0.052 | 0.05 | 0.00 |
| PRO43 | HD2 | 1.00 | 0.077 | 0.00 | 0.00 |
| PRO43 | HD3 | 1.00 | 0.003 | 1.00 | 1.37 |
| PRO43 | HB3 | 0.77 | 0.023 | 1.00 | 0.40 |

3.42.2 Detailed Probabilities of THR42CB:

Overall probability: 0.430

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR42 | 0.25 | 0.80 |
| PRO43 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T42HA | 1.00 |
| T42HG21 | 1.00 |
| T42H | 1.00 |
| T42HG1 | 1.00 |
| T42HB | 1.00 |
| P43HD3 | 0.99 |
| P43HD2 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR42 | HA | 1.00 | 0.118 | 0.00 | 0.00 |
| THR42 | HB | 1.00 | 0.293 | 0.00 | 0.00 |
| THR42 | HG21 | 1.00 | 0.518 | 0.00 | 0.00 |
| THR42 | H | 1.00 | 0.004 | 1.00 | 0.21 |
| PRO43 | HD2 | 0.99 | 0.001 | 1.00 | 1.23 |
| PRO43 | HD3 | 0.99 | 0.079 | 0.01 | 0.00 |
| PRO43 | HG2 | 0.58 | 0.000 | 1.00 | 0.23 |

3.42.3 Detailed Probabilities of THR42CG2:

Overall probability: 0.825

Overall confidence: 0.800

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR42 | 0.82 | 0.80 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T42HA | 1.00 |
| T42HB | 1.00 |
| T42HG22 | 1.00 |
| T42H | 1.00 |
| T42HG1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR42 | HA | 1.00 | 0.010 | 1.00 | 1.37 |
| THR42 | HB | 1.00 | 0.008 | 1.00 | 4.03 |
| THR42 | HG21 | 1.00 | 0.037 | 0.30 | 0.00 |
| THR42 | H | 1.00 | 0.002 | 1.00 | 0.54 |

3.42.4 Detailed Probabilities of THR42N:

Overall probability: 0.909

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO41 | 1.00 | 1.00 |
| THR42 | 1.00 | 0.80 |
| PRO43 | 0.45 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P41HB2 | 1.00 |
| P41HB3 | 1.00 |
| P41HA | 1.00 |
| T42HA | 1.00 |
| T42HB | 1.00 |
| T42HG21 | 1.00 |
| T42HG1 | 1.00 |
| T42H | 1.00 |
| P43HD2 | 1.00 |
| P43HD3 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO41 | HA | 1.00 | 0.012 | 1.00 | -515210.00 |
| PRO41 | HB2 | 1.00 | 0.011 | 1.00 | -349722.00 |
| PRO41 | HB3 | 1.00 | 0.026 | 1.00 | -1809049.00 |
| PRO41 | HG2 | 0.92 | 0.012 | 1.00 | -1809049.00 |
| PRO41 | HD2 | 0.67 | 0.008 | 1.00 | -1149313.00 |
| PRO41 | HD3 | 0.58 | 0.001 | 1.00 | -502078.00 |
| THR42 | HA | 1.00 | 0.009 | 1.00 | -1262105.00 |
| THR42 | HB | 1.00 | 0.001 | 1.00 | -399383.00 |
| THR42 | HG21 | 1.00 | 0.004 | 1.00 | -1260604.00 |
| THR42 | H | 1.00 | 0.004 | 1.00 | -24023406.00 |
| PRO43 | HD2 | 1.00 | 0.049 | 0.00 | 0.00 |
| PRO43 | HD3 | 0.99 | 0.031 | 0.90 | 0.00 |

3.42.5 Detailed Probabilities of THR42HA:

Overall probability: 0.833

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO41 | 1.00 | 1.00 |
| THR42 | 0.75 | 0.80 |
| PRO43 | 0.83 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P41HB2 | 0.98 |
| P41HA | 1.00 |
| T42HB | 1.00 |
| T42HG21 | 1.00 |
| T42H | 1.00 |
| T42HG1 | 1.00 |
| T42HA | 1.00 |
| P43HD2 | 1.00 |
| P43HD3 | 1.00 |
| P43HG2 | 0.95 |
| P43HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO41 | HA | 1.00 | 0.002 | 1.00 | 0.44 |
| PRO41 | HB2 | 0.98 | 0.027 | 1.00 | 0.10 |
| THR42 | HA | 1.00 | 0.003 | 1.00 | 7.68 |
| THR42 | HB | 1.00 | 0.118 | 0.00 | 0.00 |
| THR42 | HG21 | 1.00 | 0.010 | 1.00 | 1.37 |
| THR42 | H | 1.00 | 0.009 | 1.00 | -1262105.00 |
| PRO43 | HA | 1.00 | 0.003 | 1.00 | 0.06 |
| PRO43 | HG2 | 0.95 | 0.010 | 1.00 | 0.20 |
| PRO43 | HD2 | 1.00 | 0.005 | 1.00 | 0.80 |
| PRO43 | HD3 | 1.00 | 0.093 | 0.00 | 0.00 |
| PRO43 | HB3 | 0.77 | 0.001 | 1.00 | 0.06 |
| PRO43 | HG3 | 0.94 | 0.001 | 1.00 | 0.13 |

3.42.6 Detailed Probabilities of THR42HB:

Overall probability: 0.779

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR42 | 0.75 | 0.80 |
| PRO43 | 0.80 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T42HA | 1.00 |
| T42HG21 | 1.00 |
| T42H | 1.00 |
| T42HG1 | 1.00 |
| T42HB | 1.00 |
| P43HD3 | 0.99 |
| P43HD2 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR42 | HA | 1.00 | 0.001 | 1.00 | 1.11 |
| THR42 | HB | 1.00 | 0.293 | 0.00 | 0.00 |
| THR42 | HG21 | 1.00 | 0.008 | 1.00 | 4.03 |
| THR42 | H | 1.00 | 0.001 | 1.00 | -399383.00 |
| PRO43 | HD2 | 0.99 | 0.001 | 1.00 | 0.77 |
| PRO43 | HD3 | 0.99 | 0.116 | 0.01 | 0.00 |
| PRO43 | HA | 0.83 | 0.000 | 1.00 | 0.06 |
| PRO43 | HG2 | 0.58 | 0.012 | 1.00 | 0.17 |
| PRO43 | HG3 | 0.52 | 0.007 | 1.00 | 0.14 |

3.42.7 Detailed Probabilities of THR42HG21:

Overall probability: 0.575

Overall confidence: 0.800

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR42 | 0.58 | 0.80 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T42HA | 1.00 |
| T42HB | 1.00 |
| T42HG22 | 1.00 |
| T42H | 1.00 |
| T42HG1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR42 | HA | 1.00 | 0.004 | 1.00 | 1.19 |
| THR42 | HB | 1.00 | 0.518 | 0.00 | 0.00 |
| THR42 | HG21 | 1.00 | 0.037 | 0.30 | 0.00 |
| THR42 | H | 1.00 | 0.004 | 1.00 | -1260604.00 |

3.42.8 Detailed Probabilities of THR42H:

Overall probability: 0.768

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO41 | 0.87 | 1.00 |
| THR42 | 1.00 | 0.80 |
| PRO43 | 0.01 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P41HB2 | 1.00 |
| P41HB3 | 1.00 |
| P41HA | 1.00 |
| T42HA | 1.00 |
| T42HB | 1.00 |
| T42HG21 | 1.00 |
| T42HG1 | 1.00 |
| T42H | 1.00 |
| P43HD2 | 1.00 |
| P43HD3 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO41 | HA | 1.00 | 0.038 | 0.20 | 0.00 |
| PRO41 | HB2 | 1.00 | 0.002 | 1.00 | 0.19 |
| PRO41 | HB3 | 1.00 | 0.005 | 1.00 | 0.29 |
| PRO41 | HG2 | 0.92 | 0.004 | 1.00 | 0.56 |
| PRO41 | HD2 | 0.67 | 0.008 | 1.00 | 0.35 |
| PRO41 | HD3 | 0.58 | 0.009 | 1.00 | 0.22 |
| THR42 | HA | 1.00 | 0.006 | 1.00 | 0.66 |
| THR42 | HB | 1.00 | 0.004 | 1.00 | 0.21 |
| THR42 | HG21 | 1.00 | 0.002 | 1.00 | 0.54 |
| THR42 | H | 1.00 | 0.004 | 1.00 | -24023406.00 |
| PRO43 | HD2 | 1.00 | 0.117 | 0.00 | 0.00 |
| PRO43 | HD3 | 0.99 | 0.314 | 0.01 | 0.00 |

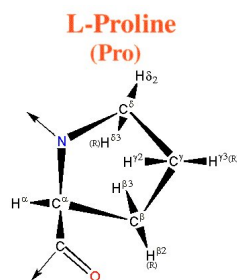
3.43 PRO(43)

Figure 33: Image from the BMRB

Residue probability: 0.804

Residue probability confidence: 0.950

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | NA | – | – | 0.000 | 0.000 |
| CA 3.43.1 | 63.797 | 62.931 | 15.301 | 0.900 | 0.900 |
| CB 3.43.2 | 30.985 | 33.632 | 13.629 | 1.000 | 0.889 |
| CG 3.43.3 | 26.838 | 28.412 | 13.801 | 0.889 | 1.000 |
| CD 3.43.4 | 50.034 | 49.797 | 3.175 | 0.846 | 1.000 |
| N | NA | – | – | 0.000 | 0.000 |
| HA 3.43.5 | 2.776 | 4.332 | 0.427 | 0.889 | 0.900 |
| HB2 3.43.6 | 1.664 | 2.099 | 0.501 | 0.825 | 0.889 |
| HB3 3.43.7 | 1.818 | 2.052 | 0.596 | 0.614 | 0.875 |
| HG2 3.43.8 | 1.982 | 1.927 | 0.364 | 0.672 | 1.000 |
| HG3 3.43.9 | 1.656 | 1.907 | 0.417 | 0.857 | 1.000 |
| HD2 3.43.10 | 3.708 | 3.640 | 0.682 | 0.546 | 1.000 |
| HD3 3.43.11 | 3.628 | 3.558 | 0.522 | 0.810 | 1.000 |

3.43.1 Detailed Probabilities of PRO43CA:

Overall probability: 0.900

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR42 | 1.00 | 1.00 |
| PRO43 | 1.00 | 1.00 |
| ALA44 | 0.00 | 0.50 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T42HA | 1.00 |
| P43HB2 | 1.00 |
| P43HB3 | 1.00 |
| P43HG2 | 1.00 |
| P43HG3 | 1.00 |
| P43HD2 | 1.00 |
| P43HD3 | 1.00 |
| P43HA | 1.00 |
| A44H | 1.00 |
| A44HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR42 | HA | 1.00 | 0.003 | 1.00 | 0.06 |
| THR42 | HB | 0.83 | 0.000 | 1.00 | 0.06 |
| PRO43 | HA | 1.00 | 0.004 | 1.00 | 5.08 |
| PRO43 | HB2 | 1.00 | 0.005 | 1.00 | 0.75 |
| PRO43 | HB3 | 1.00 | 0.007 | 1.00 | 0.72 |
| PRO43 | HG2 | 1.00 | 0.009 | 1.00 | 0.19 |
| PRO43 | HG3 | 1.00 | 0.003 | 1.00 | 0.75 |
| PRO43 | HD2 | 1.00 | 0.008 | 1.00 | 0.06 |
| PRO43 | HD3 | 1.00 | 0.004 | 1.00 | 0.09 |
| ALA44 | HA | 1.00 | 0.306 | 0.00 | 0.00 |

3.43.2 Detailed Probabilities of PRO43CB:

Overall probability: 1.000

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO43 | 1.00 | 1.00 |
| ALA44 | 1.00 | 0.50 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P43HA | 1.00 |
| P43HB3 | 1.00 |
| P43HG2 | 1.00 |
| P43HG3 | 1.00 |
| P43HD2 | 1.00 |
| P43HD3 | 1.00 |
| P43HB2 | 1.00 |
| A44H | 1.00 |
| A44HA | 0.98 |

NOESY contacts detailed probability

3.43 PRO(43)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO43 | HA | 1.00 | 0.000 | 1.00 | 0.49 |
| PRO43 | HB2 | 1.00 | 0.006 | 1.00 | 3.83 |
| PRO43 | HB3 | 1.00 | 0.008 | 1.00 | 1.85 |
| PRO43 | HG2 | 1.00 | 0.007 | 1.00 | 1.09 |
| PRO43 | HG3 | 1.00 | 0.002 | 1.00 | 3.83 |
| PRO43 | HD2 | 1.00 | 0.003 | 1.00 | 0.22 |
| PRO43 | HD3 | 1.00 | 0.004 | 1.00 | 0.20 |
| ALA44 | HA | 0.98 | 0.000 | 1.00 | 0.05 |

3.43.3 Detailed Probabilities of PRO43CG:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR42 | 1.00 | 1.00 |
| PRO43 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T42HA | 0.95 |
| P43HA | 1.00 |
| P43HB2 | 1.00 |
| P43HB3 | 1.00 |
| P43HG3 | 1.00 |
| P43HD2 | 1.00 |
| P43HD3 | 1.00 |
| P43HG2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR42 | HA | 0.95 | 0.010 | 1.00 | 0.20 |
| THR42 | HB | 0.58 | 0.012 | 1.00 | 0.17 |
| PRO43 | HA | 1.00 | 0.003 | 1.00 | 0.25 |
| PRO43 | HB2 | 1.00 | 0.022 | 1.00 | 3.12 |
| PRO43 | HB3 | 1.00 | 0.008 | 1.00 | 1.67 |
| PRO43 | HG2 | 1.00 | 0.015 | 1.00 | 12.54 |
| PRO43 | HG3 | 1.00 | 0.030 | 1.00 | 0.00 |
| PRO43 | HD2 | 1.00 | 0.793 | 0.00 | 0.00 |
| PRO43 | HD3 | 1.00 | 0.025 | 1.00 | 0.56 |

3.43.4 Detailed Probabilities of PRO43CD:

Overall probability: 0.846

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR42 | 0.75 | 1.00 |
| PRO43 | 0.90 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T42H | 1.00 |
| T42HB | 0.99 |
| T42HA | 1.00 |
| P43HA | 1.00 |
| P43HB2 | 1.00 |
| P43HB3 | 1.00 |
| P43HG2 | 1.00 |
| P43HG3 | 1.00 |
| P43HD3 | 1.00 |
| P43HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR42 | HA | 1.00 | 0.005 | 1.00 | 0.80 |
| THR42 | HB | 0.99 | 0.001 | 1.00 | 0.77 |
| THR42 | H | 1.00 | 0.117 | 0.00 | 0.00 |
| THR42 | HG21 | 0.94 | 0.000 | 1.00 | 0.33 |
| PRO43 | HA | 1.00 | 0.005 | 1.00 | 0.08 |
| PRO43 | HB2 | 1.00 | 0.005 | 1.00 | 0.52 |
| PRO43 | HB3 | 1.00 | 0.037 | 0.30 | 0.00 |
| PRO43 | HG2 | 1.00 | 0.008 | 1.00 | 0.65 |
| PRO43 | HG3 | 1.00 | 0.003 | 1.00 | 0.52 |
| PRO43 | HD2 | 1.00 | 0.005 | 1.00 | 2.33 |
| PRO43 | HD3 | 1.00 | 0.009 | 1.00 | 2.20 |

3.43.5 Detailed Probabilities of PRO43HA:

Overall probability: 0.889

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR42 | 1.00 | 1.00 |
| PRO43 | 1.00 | 1.00 |
| ALA44 | 0.00 | 0.50 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T42HA | 1.00 |
| P43HB2 | 1.00 |
| P43HB3 | 1.00 |
| P43HG2 | 1.00 |
| P43HG3 | 1.00 |
| P43HD2 | 1.00 |
| P43HD3 | 1.00 |
| P43HA | 1.00 |
| A44H | 1.00 |
| A44HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR42 | HA | 1.00 | 0.024 | 1.00 | 0.18 |
| PRO43 | HA | 1.00 | 0.004 | 1.00 | 5.08 |
| PRO43 | HB2 | 1.00 | 0.000 | 1.00 | 0.49 |
| PRO43 | HB3 | 1.00 | 0.000 | 1.00 | 0.67 |
| PRO43 | HG2 | 1.00 | 0.003 | 1.00 | 0.25 |
| PRO43 | HG3 | 1.00 | 0.006 | 1.00 | 0.29 |
| PRO43 | HD2 | 1.00 | 0.005 | 1.00 | 0.08 |
| PRO43 | HD3 | 1.00 | 0.005 | 1.00 | 0.09 |
| ALA44 | HA | 1.00 | 0.343 | 0.00 | 0.00 |

3.43.6 Detailed Probabilities of PRO43HB2:

Overall probability: 0.825

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO43 | 0.86 | 1.00 |
| ALA44 | 0.60 | 0.50 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P43HA | 1.00 |
| P43HB3 | 1.00 |
| P43HG2 | 1.00 |
| P43HG3 | 1.00 |
| P43HD2 | 1.00 |
| P43HD3 | 1.00 |
| P43HB2 | 1.00 |
| A44H | 1.00 |
| A44HA | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO43 | HA | 1.00 | 0.005 | 1.00 | 0.75 |
| PRO43 | HB2 | 1.00 | 0.006 | 1.00 | 3.83 |
| PRO43 | HB3 | 1.00 | 0.004 | 1.00 | 2.71 |
| PRO43 | HG2 | 1.00 | 0.022 | 1.00 | 3.12 |
| PRO43 | HG3 | 1.00 | 0.147 | 0.00 | 0.00 |
| PRO43 | HD2 | 1.00 | 0.005 | 1.00 | 0.52 |
| PRO43 | HD3 | 1.00 | 0.005 | 1.00 | 0.55 |
| ALA44 | HA | 0.98 | 0.034 | 0.60 | 0.00 |

3.43.7 Detailed Probabilities of PRO43HB3:

Overall probability: 0.614

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO43 | 0.61 | 1.00 |
| ALA44 | 0.00 | 0.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P43HA | 1.00 |
| P43HB2 | 1.00 |
| P43HG2 | 1.00 |
| P43HG3 | 1.00 |
| P43HD2 | 1.00 |
| P43HD3 | 1.00 |
| P43HB3 | 1.00 |
| A44H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO43 | HA | 1.00 | 0.007 | 1.00 | 0.72 |
| PRO43 | HB2 | 1.00 | 0.008 | 1.00 | 1.85 |
| PRO43 | HB3 | 1.00 | 0.158 | 0.00 | 0.00 |
| PRO43 | HG2 | 1.00 | 0.008 | 1.00 | 1.67 |
| PRO43 | HG3 | 1.00 | 0.007 | 1.00 | 1.11 |
| PRO43 | HD2 | 1.00 | 0.037 | 0.30 | 0.00 |
| PRO43 | HD3 | 1.00 | 0.149 | 0.00 | 0.00 |

3.43.8 Detailed Probabilities of PRO43HG2:

Overall probability: 0.672

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR42 | 0.52 | 1.00 |
| PRO43 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T42HA | 0.95 |
| P43HA | 1.00 |
| P43HB2 | 1.00 |
| P43HB3 | 1.00 |
| P43HG3 | 1.00 |
| P43HD2 | 1.00 |
| P43HD3 | 1.00 |
| P43HG2 | 1.00 |

NOESY contacts detailed probability

3.43 PRO(43)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR42 | HA | 0.95 | 0.052 | 0.05 | 0.00 |
| THR42 | HB | 0.58 | 0.000 | 1.00 | 0.23 |
| PRO43 | HA | 1.00 | 0.009 | 1.00 | 0.19 |
| PRO43 | HB2 | 1.00 | 0.007 | 1.00 | 1.09 |
| PRO43 | HB3 | 1.00 | 0.322 | 0.00 | 0.00 |
| PRO43 | HG2 | 1.00 | 0.015 | 1.00 | 12.54 |
| PRO43 | HG3 | 1.00 | 0.171 | 0.00 | 0.00 |
| PRO43 | HD2 | 1.00 | 0.008 | 1.00 | 0.65 |
| PRO43 | HD3 | 1.00 | 0.015 | 1.00 | 1.33 |

3.43.9 Detailed Probabilities of PRO43HG3:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO43 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P43HA | 1.00 |
| P43HB2 | 1.00 |
| P43HB3 | 1.00 |
| P43HG2 | 1.00 |
| P43HD2 | 1.00 |
| P43HD3 | 1.00 |
| P43HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO43 | HA | 1.00 | 0.003 | 1.00 | 0.75 |
| PRO43 | HB2 | 1.00 | 0.002 | 1.00 | 3.83 |
| PRO43 | HB3 | 1.00 | 0.004 | 1.00 | 2.71 |
| PRO43 | HG2 | 1.00 | 0.030 | 1.00 | 0.00 |
| PRO43 | HG3 | 1.00 | 0.155 | 0.00 | 0.00 |
| PRO43 | HD2 | 1.00 | 0.003 | 1.00 | 0.52 |
| PRO43 | HD3 | 1.00 | 0.003 | 1.00 | 0.55 |

3.43.10 Detailed Probabilities of PRO43HD2:

Overall probability: 0.546

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR42 | 0.50 | 1.00 |
| PRO43 | 0.57 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T42H | 1.00 |
| T42HB | 0.99 |
| T42HA | 1.00 |
| P43HA | 1.00 |
| P43HB2 | 1.00 |
| P43HB3 | 1.00 |
| P43HG2 | 1.00 |
| P43HG3 | 1.00 |
| P43HD3 | 1.00 |
| P43HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR42 | HA | 1.00 | 0.077 | 0.00 | 0.00 |
| THR42 | HB | 0.99 | 0.001 | 1.00 | 1.23 |
| THR42 | H | 1.00 | 0.049 | 0.00 | 0.00 |
| THR42 | HG21 | 0.94 | 0.002 | 1.00 | 0.40 |
| PRO43 | HA | 1.00 | 0.008 | 1.00 | 0.06 |
| PRO43 | HB2 | 1.00 | 0.003 | 1.00 | 0.22 |
| PRO43 | HB3 | 1.00 | 0.503 | 0.00 | 0.00 |
| PRO43 | HG2 | 1.00 | 0.793 | 0.00 | 0.00 |
| PRO43 | HG3 | 1.00 | 0.005 | 1.00 | 0.35 |
| PRO43 | HD2 | 1.00 | 0.005 | 1.00 | 2.33 |
| PRO43 | HD3 | 1.00 | 0.051 | 0.00 | 0.00 |

3.43.11 Detailed Probabilities of PRO43HD3:

Overall probability: 0.810

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR42 | 0.73 | 1.00 |
| PRO43 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T42HB | 0.99 |
| T42H | 0.99 |
| T42HA | 1.00 |
| P43HA | 1.00 |
| P43HB2 | 1.00 |
| P43HB3 | 1.00 |
| P43HG2 | 1.00 |
| P43HG3 | 1.00 |
| P43HD2 | 1.00 |
| P43HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR42 | HA | 1.00 | 0.003 | 1.00 | 1.37 |
| THR42 | HB | 0.99 | 0.079 | 0.01 | 0.00 |
| THR42 | H | 0.99 | 0.031 | 0.90 | 0.00 |
| THR42 | HG21 | 0.79 | 0.011 | 1.00 | 0.41 |
| PRO43 | HA | 1.00 | 0.004 | 1.00 | 0.09 |
| PRO43 | HB2 | 1.00 | 0.004 | 1.00 | 0.20 |
| PRO43 | HB3 | 1.00 | 0.423 | 0.00 | 0.00 |
| PRO43 | HG2 | 1.00 | 0.025 | 1.00 | 0.56 |
| PRO43 | HG3 | 1.00 | 0.000 | 1.00 | 0.39 |
| PRO43 | HD2 | 1.00 | 0.009 | 1.00 | 2.20 |
| PRO43 | HD3 | 1.00 | 0.029 | 1.00 | 5.13 |

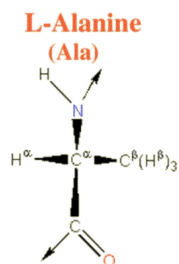
3.44 ALA(44)

Figure 34: Image from the BMRB

Residue probability: 0.867

Residue probability confidence: 0.804

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-----------|-------------|---------|--------|---------------------|--------------------|
| CA 3.44.1 | 54.577 | 53.289 | 3.425 | 0.767 | 0.857 |
| CB 3.44.2 | 17.814 | 19.355 | 4.103 | 1.000 | 0.750 |
| N | NA | - | - | 0.000 | 0.000 |
| HA 3.44.3 | 4.006 | 4.254 | 0.459 | 0.700 | 0.857 |
| HB 3.44.4 | 1.327 | 1.346 | 0.258 | 1.000 | 0.750 |
| H | NA | - | - | 0.000 | 0.000 |

3.44.1 Detailed Probabilities of ALA44CA:

Overall probability: 0.767

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO43 | 0.30 | 1.00 |
| ALA44 | 1.00 | 0.67 |
| ALA45 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P43HA | 1.00 |
| P43HB2 | 0.98 |
| A44H | 1.00 |
| A44HB1 | 1.00 |
| A44HA | 1.00 |
| A45H | 1.00 |
| A45HA | 1.00 |

NOESY contacts detailed probability

3.44 ALA(44)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO43 | HA | 1.00 | 0.343 | 0.00 | 0.00 |
| PRO43 | HB2 | 0.98 | 0.034 | 0.60 | 0.00 |
| ALA44 | HA | 1.00 | 0.001 | 1.00 | 17.41 |
| ALA44 | HB1 | 1.00 | 0.000 | 1.00 | 4.41 |
| ALA45 | HA | 1.00 | 0.016 | 1.00 | 0.06 |
| ALA45 | H | 1.00 | 0.003 | 1.00 | 0.27 |

3.44.2 Detailed Probabilities of ALA44CB:

Overall probability: 1.000

Overall confidence: 0.750

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA44 | 1.00 | 0.67 |
| ALA45 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A44HA | 1.00 |
| A44H | 1.00 |
| A44HB2 | 1.00 |
| A45H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA44 | HA | 1.00 | 0.001 | 1.00 | 4.56 |
| ALA44 | HB1 | 1.00 | 0.000 | 1.00 | 88.98 |
| ALA45 | H | 1.00 | 0.002 | 1.00 | 0.98 |
| ALA45 | HA | 0.70 | 0.012 | 1.00 | 0.41 |

3.44.3 Detailed Probabilities of ALA44HA:

Overall probability: 0.700

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO43 | 0.50 | 1.00 |
| ALA44 | 1.00 | 0.67 |
| ALA45 | 0.60 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P43HA | 1.00 |
| P43HB2 | 0.98 |
| A44H | 1.00 |
| A44HB1 | 1.00 |
| A44HA | 1.00 |
| A45H | 1.00 |
| A45HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO43 | HA | 1.00 | 0.306 | 0.00 | 0.00 |
| PRO43 | HB2 | 0.98 | 0.000 | 1.00 | 0.05 |
| ALA44 | HA | 1.00 | 0.001 | 1.00 | 17.41 |
| ALA44 | HB1 | 1.00 | 0.001 | 1.00 | 4.56 |
| ALA45 | HA | 1.00 | 0.038 | 0.20 | 0.00 |
| ALA45 | H | 1.00 | 0.003 | 1.00 | -542499.00 |

3.44.4 Detailed Probabilities of ALA44HB1:

Overall probability: 1.000

Overall confidence: 0.750

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA44 | 1.00 | 0.67 |
| ALA45 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A44HA | 1.00 |
| A44H | 1.00 |
| A44HB2 | 1.00 |
| A45H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA44 | HA | 1.00 | 0.000 | 1.00 | 4.41 |
| ALA44 | HB1 | 1.00 | 0.000 | 1.00 | 88.98 |
| ALA45 | H | 1.00 | 0.005 | 1.00 | -2035050.00 |
| ALA45 | HA | 0.70 | 0.001 | 1.00 | 0.20 |

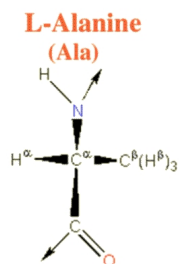
3.45 ALA(45)

Figure 35: Image from the BMRB

Residue probability: 0.957

Residue probability confidence: 0.952

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-----------|-------------|---------|--------|---------------------|--------------------|
| CA 3.45.1 | 52.958 | 53.289 | 3.425 | 0.886 | 1.000 |
| CB 3.45.2 | 18.752 | 19.355 | 4.103 | 1.000 | 1.000 |
| N 3.45.3 | 118.829 | 123.100 | 4.487 | 1.000 | 0.857 |
| HA 3.45.4 | 4.466 | 4.254 | 0.459 | 0.857 | 1.000 |
| HB 3.45.5 | 1.745 | 1.346 | 0.258 | 1.000 | 1.000 |
| H 3.45.6 | 7.737 | 8.206 | 0.601 | 1.000 | 0.857 |

3.45.1 Detailed Probabilities of ALA45CA:

Overall probability: 0.886

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA44 | 0.60 | 1.00 |
| ALA45 | 1.00 | 1.00 |
| ALA46 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A44HA | 1.00 |
| A45H | 1.00 |
| A45HB1 | 1.00 |
| A45HA | 1.00 |
| A46H | 1.00 |
| A46HA | 1.00 |

NOESY contacts detailed probability

3.45 ALA(45)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA44 | HA | 1.00 | 0.038 | 0.20 | 0.00 |
| ALA44 | HB1 | 0.67 | 0.001 | 1.00 | 0.20 |
| ALA45 | HA | 1.00 | 0.002 | 1.00 | 12.48 |
| ALA45 | HB1 | 1.00 | 0.005 | 1.00 | 2.99 |
| ALA45 | H | 1.00 | 0.007 | 1.00 | 0.71 |
| ALA46 | HA | 1.00 | 0.013 | 1.00 | 0.07 |
| ALA46 | H | 1.00 | 0.001 | 1.00 | 0.38 |

3.45.2 Detailed Probabilities of ALA45CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA45 | 1.00 | 1.00 |
| ALA46 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A45HA | 1.00 |
| A45H | 1.00 |
| A45HB2 | 1.00 |
| A46H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA45 | HA | 1.00 | 0.000 | 1.00 | 2.43 |
| ALA45 | HB1 | 1.00 | 0.005 | 1.00 | 46.48 |
| ALA45 | H | 1.00 | 0.004 | 1.00 | 1.75 |
| ALA46 | H | 1.00 | 0.002 | 1.00 | 0.54 |
| ALA46 | HA | 0.70 | 0.006 | 1.00 | 0.16 |

3.45.3 Detailed Probabilities of ALA45N:

Overall probability: 1.000

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA44 | 1.00 | 0.67 |
| ALA45 | 1.00 | 1.00 |
| ALA46 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A44HB2 | 1.00 |
| A44H | 1.00 |
| A44HA | 1.00 |
| A45HA | 1.00 |
| A45HB1 | 1.00 |
| A45H | 1.00 |
| A46H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA44 | HA | 1.00 | 0.003 | 1.00 | -542499.00 |
| ALA44 | HB1 | 1.00 | 0.005 | 1.00 | -2035050.00 |
| ALA45 | HA | 1.00 | 0.001 | 1.00 | -1692257.00 |
| ALA45 | HB1 | 1.00 | 0.006 | 1.00 | -4747742.00 |
| ALA45 | H | 1.00 | 0.005 | 1.00 | -17988808.00 |
| ALA46 | H | 1.00 | 0.006 | 1.00 | -1809153.00 |

3.45.4 Detailed Probabilities of ALA45HA:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA44 | 1.00 | 1.00 |
| ALA45 | 1.00 | 1.00 |
| ALA46 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A44HA | 1.00 |
| A45H | 1.00 |
| A45HB1 | 1.00 |
| A45HA | 1.00 |
| A46H | 1.00 |
| A46HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA44 | HA | 1.00 | 0.016 | 1.00 | 0.06 |
| ALA44 | HB1 | 0.67 | 0.012 | 1.00 | 0.41 |
| ALA45 | HA | 1.00 | 0.002 | 1.00 | 12.48 |
| ALA45 | HB1 | 1.00 | 0.000 | 1.00 | 2.43 |
| ALA45 | H | 1.00 | 0.001 | 1.00 | -1692257.00 |
| ALA46 | HA | 1.00 | 0.267 | 0.00 | 0.00 |
| ALA46 | H | 1.00 | 0.002 | 1.00 | -672903.00 |

3.45.5 Detailed Probabilities of ALA45HB1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA45 | 1.00 | 1.00 |
| ALA46 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A45HA | 1.00 |
| A45H | 1.00 |
| A45HB2 | 1.00 |
| A46H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA45 | HA | 1.00 | 0.005 | 1.00 | 2.99 |
| ALA45 | HB1 | 1.00 | 0.005 | 1.00 | 46.48 |
| ALA45 | H | 1.00 | 0.006 | 1.00 | -4747742.00 |
| ALA46 | H | 1.00 | 0.006 | 1.00 | -1326677.00 |
| ALA46 | HA | 0.70 | 0.007 | 1.00 | 0.15 |

3.45.6 Detailed Probabilities of ALA45H:

Overall probability: 1.000

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA44 | 1.00 | 0.67 |
| ALA45 | 1.00 | 1.00 |
| ALA46 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A44HB2 | 1.00 |
| A44H | 1.00 |
| A44HA | 1.00 |
| A45HA | 1.00 |
| A45HB1 | 1.00 |
| A45H | 1.00 |
| A46H | 1.00 |

NOESY contacts detailed probability

3.45 ALA(45)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA44 | HA | 1.00 | 0.003 | 1.00 | 0.27 |
| ALA44 | HB1 | 1.00 | 0.002 | 1.00 | 0.98 |
| ALA45 | HA | 1.00 | 0.007 | 1.00 | 0.71 |
| ALA45 | HB1 | 1.00 | 0.004 | 1.00 | 1.75 |
| ALA45 | H | 1.00 | 0.005 | 1.00 | -17988808.00 |
| ALA46 | H | 1.00 | 0.027 | 1.00 | -1845334.00 |
| ALA46 | HA | 0.88 | 0.019 | 1.00 | 0.16 |
| ALA46 | HB1 | 0.52 | 0.009 | 1.00 | 0.26 |

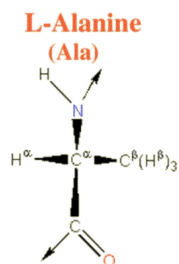
3.46 ALA(46)

Figure 36: Image from the BMRB

Residue probability: 0.955

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-----------|-------------|---------|--------|---------------------|--------------------|
| CA 3.46.1 | 52.906 | 53.289 | 3.425 | 0.875 | 1.000 |
| CB 3.46.2 | 18.635 | 19.355 | 4.103 | 1.000 | 1.000 |
| N 3.46.3 | 118.013 | 123.100 | 4.487 | 1.000 | 1.000 |
| HA 3.46.4 | 4.057 | 4.254 | 0.459 | 0.857 | 1.000 |
| HB 3.46.5 | 1.289 | 1.346 | 0.258 | 1.000 | 1.000 |
| H 3.46.6 | 7.618 | 8.206 | 0.601 | 1.000 | 1.000 |

3.46.1 Detailed Probabilities of ALA46CA:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA45 | 0.67 | 1.00 |
| ALA46 | 1.00 | 1.00 |
| PHE47 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A45HA | 1.00 |
| A46H | 1.00 |
| A46HB1 | 1.00 |
| A46HA | 1.00 |
| F47HA | 1.00 |
| F47H | 1.00 |

NOESY contacts detailed probability

3.46 ALA(46)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA45 | HA | 1.00 | 0.267 | 0.00 | 0.00 |
| ALA45 | HB1 | 0.67 | 0.007 | 1.00 | 0.15 |
| ALA45 | H | 0.88 | 0.019 | 1.00 | 0.16 |
| ALA46 | HA | 1.00 | 0.000 | 1.00 | 5.75 |
| ALA46 | HB1 | 1.00 | 0.001 | 1.00 | 1.43 |
| ALA46 | H | 1.00 | 0.004 | 1.00 | 0.49 |
| PHE47 | HA | 1.00 | 0.011 | 1.00 | 0.12 |
| PHE47 | H | 1.00 | 0.001 | 1.00 | 0.14 |

3.46.2 Detailed Probabilities of ALA46CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA46 | 1.00 | 1.00 |
| PHE47 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A46HA | 1.00 |
| A46H | 1.00 |
| A46HB2 | 1.00 |
| F47H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA46 | HA | 1.00 | 0.000 | 1.00 | 1.43 |
| ALA46 | HB1 | 1.00 | 0.001 | 1.00 | 27.66 |
| ALA46 | H | 1.00 | 0.003 | 1.00 | 1.60 |
| PHE47 | H | 1.00 | 0.005 | 1.00 | 0.22 |
| PHE47 | HA | 0.72 | 0.017 | 1.00 | 0.11 |

3.46.3 Detailed Probabilities of ALA46N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA45 | 1.00 | 1.00 |
| ALA46 | 1.00 | 1.00 |
| PHE47 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A45HB2 | 1.00 |
| A45H | 1.00 |
| A45HA | 1.00 |
| A46HA | 1.00 |
| A46HB1 | 1.00 |
| A46H | 1.00 |
| F47H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA45 | HA | 1.00 | 0.002 | 1.00 | -672903.00 |
| ALA45 | HB1 | 1.00 | 0.006 | 1.00 | -1326677.00 |
| ALA45 | H | 1.00 | 0.027 | 1.00 | -1845334.00 |
| ALA46 | HA | 1.00 | 0.006 | 1.00 | -1209114.00 |
| ALA46 | HB1 | 1.00 | 0.000 | 1.00 | -4093922.00 |
| ALA46 | H | 1.00 | 0.002 | 1.00 | -22693856.00 |
| PHE47 | H | 1.00 | 0.004 | 1.00 | -1339206.00 |
| PHE47 | HA | 0.90 | 0.007 | 1.00 | -135776.00 |
| PHE47 | HB2 | 0.57 | 0.010 | 1.00 | -116486.00 |

3.46.4 Detailed Probabilities of ALA46HA:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA45 | 1.00 | 1.00 |
| ALA46 | 1.00 | 1.00 |
| PHE47 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A45HA | 1.00 |
| A46H | 1.00 |
| A46HB1 | 1.00 |
| A46HA | 1.00 |
| F47HA | 1.00 |
| F47H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA45 | HA | 1.00 | 0.013 | 1.00 | 0.07 |
| ALA45 | HB1 | 0.67 | 0.006 | 1.00 | 0.16 |
| ALA46 | HA | 1.00 | 0.000 | 1.00 | 5.75 |
| ALA46 | HB1 | 1.00 | 0.000 | 1.00 | 1.43 |
| ALA46 | H | 1.00 | 0.006 | 1.00 | -1209114.00 |
| PHE47 | HA | 1.00 | 0.149 | 0.00 | 0.00 |
| PHE47 | H | 1.00 | 0.010 | 1.00 | -350186.00 |

3.46.5 Detailed Probabilities of ALA46HB1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA46 | 1.00 | 1.00 |
| PHE47 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A46HA | 1.00 |
| A46H | 1.00 |
| A46HB2 | 1.00 |
| F47H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA46 | HA | 1.00 | 0.001 | 1.00 | 1.43 |
| ALA46 | HB1 | 1.00 | 0.001 | 1.00 | 27.66 |
| ALA46 | H | 1.00 | 0.000 | 1.00 | -4093922.00 |
| PHE47 | H | 1.00 | 0.001 | 1.00 | -601574.00 |
| PHE47 | HA | 0.72 | 0.006 | 1.00 | 0.16 |

3.46.6 Detailed Probabilities of ALA46H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA45 | 1.00 | 1.00 |
| ALA46 | 1.00 | 1.00 |
| PHE47 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A45HB2 | 1.00 |
| A45H | 1.00 |
| A45HA | 1.00 |
| A46HA | 1.00 |
| A46HB1 | 1.00 |
| A46H | 1.00 |
| F47H | 1.00 |

NOESY contacts detailed probability

3.46 ALA(46)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA45 | HA | 1.00 | 0.001 | 1.00 | 0.38 |
| ALA45 | HB1 | 1.00 | 0.002 | 1.00 | 0.54 |
| ALA45 | H | 1.00 | 0.006 | 1.00 | -1809153.00 |
| ALA46 | HA | 1.00 | 0.004 | 1.00 | 0.49 |
| ALA46 | HB1 | 1.00 | 0.003 | 1.00 | 1.60 |
| ALA46 | H | 1.00 | 0.002 | 1.00 | -22693856.00 |
| PHE47 | H | 1.00 | 0.004 | 1.00 | -1042246.00 |
| PHE47 | HA | 0.90 | 0.016 | 1.00 | 0.07 |

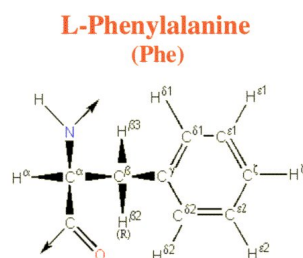
3.47 PHE(47)

Figure 37: Image from the BMRB

Residue probability: 0.751

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 175.678 | 175.508 | 2.010 | 0.000 | 0.000 |
| CA 3.47.1 | 60.106 | 58.245 | 3.808 | 0.917 | 1.000 |
| CB 3.47.2 | 38.099 | 40.078 | 3.616 | 0.889 | 1.000 |
| CD1 3.47.3 | 131.773 | 131.234 | 9.579 | 0.778 | 1.000 |
| CD2 3.47.4 | 131.956 | 131.352 | 9.581 | 0.778 | 1.000 |
| CE1 3.47.5 | 131.718 | 130.599 | 3.219 | 0.571 | 1.000 |
| CE2 3.47.6 | 131.669 | 130.633 | 2.839 | 0.571 | 1.000 |
| CZ 3.47.7 | 129.887 | 129.042 | 3.448 | 0.600 | 1.000 |
| N 3.47.8 | 116.439 | 120.315 | 4.931 | 1.000 | 1.000 |
| HA 3.47.9 | 4.210 | 4.625 | 1.237 | 0.917 | 1.000 |
| HB2 3.47.10 | 3.234 | 2.980 | 0.399 | 1.000 | 1.000 |
| HB3 3.47.11 | 3.122 | 2.916 | 0.434 | 0.900 | 1.000 |
| HD1 3.47.12 | 7.318 | 7.037 | 0.347 | 0.778 | 1.000 |
| HD2 3.47.13 | 7.318 | 7.022 | 0.417 | 0.778 | 1.000 |
| HE1 3.47.14 | 7.377 | 7.046 | 0.417 | 0.400 | 1.000 |
| HE2 3.47.15 | 7.377 | 7.043 | 0.400 | 0.286 | 1.000 |
| HZ 3.47.16 | 7.314 | 6.984 | 1.598 | 0.600 | 1.000 |
| H 3.47.17 | 7.346 | 8.375 | 0.710 | 1.000 | 1.000 |

3.47.1 Detailed Probabilities of PHE47CA:

Overall probability: 0.917

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA46 | 0.67 | 1.00 |
| PHE47 | 1.00 | 1.00 |
| ARG48 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A46HA | 1.00 |
| F47HB2 | 1.00 |
| F47HB3 | 1.00 |
| F47HD1 | 1.00 |
| F47HD2 | 1.00 |
| F47H | 1.00 |
| F47HA | 1.00 |
| R48H | 1.00 |
| R48HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA46 | HA | 1.00 | 0.149 | 0.00 | 0.00 |
| ALA46 | HB1 | 0.68 | 0.006 | 1.00 | 0.16 |
| ALA46 | H | 0.90 | 0.016 | 1.00 | 0.07 |
| PHE47 | HA | 1.00 | 0.004 | 1.00 | 10.19 |
| PHE47 | HB2 | 1.00 | 0.002 | 1.00 | 1.66 |
| PHE47 | HB3 | 1.00 | 0.001 | 1.00 | 1.80 |
| PHE47 | HD1 | 1.00 | 0.024 | 1.00 | 0.75 |
| PHE47 | HD2 | 1.00 | 0.024 | 1.00 | 0.75 |
| PHE47 | H | 1.00 | 0.004 | 1.00 | 0.75 |
| ARG48 | HA | 1.00 | 0.010 | 1.00 | 10.19 |
| ARG48 | H | 1.00 | 0.012 | 1.00 | 0.15 |
| ARG48 | HB2 | 0.50 | 0.004 | 1.00 | 0.18 |

3.47.2 Detailed Probabilities of PHE47CB:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE47 | 0.86 | 1.00 |
| ARG48 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F47HA | 1.00 |
| F47HB3 | 1.00 |
| F47HD1 | 1.00 |
| F47HD2 | 1.00 |
| F47HE2 | 1.00 |
| F47H | 1.00 |
| F47HB2 | 1.00 |
| R48H | 1.00 |

NOESY contacts detailed probability

3.47 PHE(47)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE47 | HA | 1.00 | 0.004 | 1.00 | 1.41 |
| PHE47 | HB2 | 1.00 | 0.001 | 1.00 | 5.82 |
| PHE47 | HB3 | 1.00 | 0.007 | 1.00 | 5.38 |
| PHE47 | HD1 | 1.00 | 0.008 | 1.00 | 1.23 |
| PHE47 | HD2 | 1.00 | 0.008 | 1.00 | 1.23 |
| PHE47 | HE2 | 1.00 | 0.051 | 0.00 | 0.00 |
| PHE47 | H | 1.00 | 0.020 | 1.00 | 1.23 |
| ARG48 | H | 1.00 | 0.009 | 1.00 | 0.11 |
| ARG48 | HA | 0.64 | 0.010 | 1.00 | 1.41 |

3.47.3 Detailed Probabilities of PHE47CD1:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE47 | 0.78 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F47HA | 1.00 |
| F47HB2 | 1.00 |
| F47HB3 | 1.00 |
| F47HD2 | 1.00 |
| F47HE1 | 1.00 |
| F47HE2 | 1.00 |
| F47HZ | 1.00 |
| F47H | 1.00 |
| F47HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE47 | HA | 1.00 | 0.009 | 1.00 | 0.09 |
| PHE47 | HB2 | 1.00 | 0.000 | 1.00 | 0.20 |
| PHE47 | HB3 | 1.00 | 0.004 | 1.00 | 0.85 |
| PHE47 | HD1 | 1.00 | 0.001 | 1.00 | 5.68 |
| PHE47 | HD2 | 1.00 | 0.001 | 1.00 | 5.68 |
| PHE47 | HE1 | 1.00 | 0.058 | 0.00 | 0.00 |
| PHE47 | HE2 | 1.00 | 0.058 | 0.00 | 0.00 |
| PHE47 | HZ | 1.00 | 0.002 | 1.00 | 23.43 |
| PHE47 | H | 1.00 | 0.027 | 1.00 | 5.68 |

3.47.4 Detailed Probabilities of PHE47CD2:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE47 | 0.78 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F47HA | 1.00 |
| F47HB2 | 1.00 |
| F47HB3 | 1.00 |
| F47HD1 | 1.00 |
| F47HE1 | 1.00 |
| F47HE2 | 1.00 |
| F47HZ | 1.00 |
| F47H | 0.99 |
| F47HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE47 | HA | 1.00 | 0.009 | 1.00 | 0.09 |
| PHE47 | HB2 | 1.00 | 0.000 | 1.00 | 0.20 |
| PHE47 | HB3 | 1.00 | 0.004 | 1.00 | 0.85 |
| PHE47 | HD1 | 1.00 | 0.001 | 1.00 | 5.68 |
| PHE47 | HD2 | 1.00 | 0.001 | 1.00 | 5.68 |
| PHE47 | HE1 | 1.00 | 0.058 | 0.00 | 0.00 |
| PHE47 | HE2 | 1.00 | 0.058 | 0.00 | 0.00 |
| PHE47 | HZ | 1.00 | 0.002 | 1.00 | 23.43 |
| PHE47 | H | 0.99 | 0.027 | 1.00 | 5.68 |

3.47.5 Detailed Probabilities of PHE47CE1:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE47 | 0.57 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F47HD1 | 1.00 |
| F47HD2 | 1.00 |
| F47HE2 | 1.00 |
| F47HZ | 1.00 |
| F47HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE47 | HD1 | 1.00 | 0.049 | 0.00 | 0.00 |
| PHE47 | HD2 | 1.00 | 0.049 | 0.00 | 0.00 |
| PHE47 | HE1 | 1.00 | 0.008 | 1.00 | 16.89 |
| PHE47 | HE2 | 1.00 | 0.008 | 1.00 | 16.89 |
| PHE47 | HZ | 1.00 | 0.053 | 0.00 | 0.00 |
| PHE47 | HB2 | 0.90 | 0.004 | 1.00 | 0.36 |
| PHE47 | HB3 | 0.89 | 0.001 | 1.00 | 0.11 |

3.47.6 Detailed Probabilities of PHE47CE2:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE47 | 0.57 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F47HB2 | 1.00 |
| F47HB3 | 1.00 |
| F47HD1 | 1.00 |
| F47HD2 | 1.00 |
| F47HE1 | 1.00 |
| F47HZ | 1.00 |
| F47HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE47 | HB2 | 1.00 | 0.004 | 1.00 | 0.36 |
| PHE47 | HB3 | 1.00 | 0.001 | 1.00 | 0.11 |
| PHE47 | HD1 | 1.00 | 0.049 | 0.00 | 0.00 |
| PHE47 | HD2 | 1.00 | 0.049 | 0.00 | 0.00 |
| PHE47 | HE1 | 1.00 | 0.008 | 1.00 | 16.89 |
| PHE47 | HE2 | 1.00 | 0.008 | 1.00 | 16.89 |
| PHE47 | HZ | 1.00 | 0.053 | 0.00 | 0.00 |

3.47.7 Detailed Probabilities of PHE47CZ:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE47 | 0.60 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F47HD1 | 1.00 |
| F47HD2 | 1.00 |
| F47HE1 | 1.00 |
| F47HE2 | 1.00 |
| F47HZ | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE47 | HD1 | 1.00 | 0.012 | 1.00 | 20.18 |
| PHE47 | HD2 | 1.00 | 0.012 | 1.00 | 20.18 |
| PHE47 | HE1 | 1.00 | 0.044 | 0.00 | 0.00 |
| PHE47 | HE2 | 1.00 | 0.044 | 0.00 | 0.00 |
| PHE47 | HZ | 1.00 | 0.016 | 1.00 | 20.18 |

3.47.8 Detailed Probabilities of PHE47N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA46 | 1.00 | 1.00 |
| PHE47 | 1.00 | 1.00 |
| ARG48 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A46HA | 1.00 |
| A46HB1 | 1.00 |
| A46H | 1.00 |
| F47HA | 1.00 |
| F47HB2 | 1.00 |
| F47HB3 | 1.00 |
| F47HD1 | 1.00 |
| F47HD2 | 0.99 |
| F47H | 1.00 |
| R48H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA46 | HA | 1.00 | 0.010 | 1.00 | -350186.00 |
| ALA46 | HB1 | 1.00 | 0.001 | 1.00 | -601574.00 |
| ALA46 | H | 1.00 | 0.004 | 1.00 | -1042246.00 |
| PHE47 | HA | 1.00 | 0.004 | 1.00 | -1103594.00 |
| PHE47 | HB2 | 1.00 | 0.000 | 1.00 | -1139898.00 |
| PHE47 | HB3 | 1.00 | 0.004 | 1.00 | -1597845.00 |
| PHE47 | HD1 | 1.00 | 0.030 | 1.00 | 0.00 |
| PHE47 | HD2 | 0.99 | 0.030 | 1.00 | 0.00 |
| PHE47 | H | 1.00 | 0.002 | 1.00 | -9285072.00 |
| ARG48 | H | 1.00 | 0.002 | 1.00 | -460786.00 |
| ARG48 | HA | 0.90 | 0.010 | 1.00 | -1103594.00 |

3.47.9 Detailed Probabilities of PHE47HA:

Overall probability: 0.917

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA46 | 1.00 | 1.00 |
| PHE47 | 1.00 | 1.00 |
| ARG48 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A46HA | 1.00 |
| F47HB2 | 1.00 |
| F47HB3 | 1.00 |
| F47HD1 | 1.00 |
| F47HD2 | 1.00 |
| F47H | 1.00 |
| F47HA | 1.00 |
| R48H | 1.00 |
| R48HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA46 | HA | 1.00 | 0.011 | 1.00 | 0.12 |
| ALA46 | HB1 | 0.68 | 0.017 | 1.00 | 0.11 |
| ALA46 | H | 0.90 | 0.007 | 1.00 | -135776.00 |
| PHE47 | HA | 1.00 | 0.004 | 1.00 | 10.19 |
| PHE47 | HB2 | 1.00 | 0.004 | 1.00 | 1.41 |
| PHE47 | HB3 | 1.00 | 0.004 | 1.00 | 1.26 |
| PHE47 | HD1 | 1.00 | 0.009 | 1.00 | 0.09 |
| PHE47 | HD2 | 1.00 | 0.009 | 1.00 | 0.09 |
| PHE47 | H | 1.00 | 0.004 | 1.00 | -1103594.00 |
| ARG48 | HA | 1.00 | 0.214 | 0.00 | 0.00 |
| ARG48 | H | 1.00 | 0.004 | 1.00 | -967450.00 |
| ARG48 | HB2 | 0.50 | 0.009 | 1.00 | 1.00 |

3.47.10 Detailed Probabilities of PHE47HB2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE47 | 1.00 | 1.00 |
| ARG48 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F47HA | 1.00 |
| F47HB3 | 1.00 |
| F47HD1 | 1.00 |
| F47HD2 | 1.00 |
| F47HE2 | 1.00 |
| F47H | 1.00 |
| F47HB2 | 1.00 |
| R48H | 1.00 |

NOESY contacts detailed probability

3.47 PHE(47)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE47 | HA | 1.00 | 0.002 | 1.00 | 1.66 |
| PHE47 | HB2 | 1.00 | 0.001 | 1.00 | 5.82 |
| PHE47 | HB3 | 1.00 | 0.001 | 1.00 | 4.85 |
| PHE47 | HD1 | 1.00 | 0.000 | 1.00 | 0.20 |
| PHE47 | HD2 | 1.00 | 0.000 | 1.00 | 0.20 |
| PHE47 | HE2 | 1.00 | 0.004 | 1.00 | 0.36 |
| PHE47 | H | 1.00 | 0.000 | 1.00 | -1139898.00 |
| PHE47 | HE1 | 0.90 | 0.004 | 1.00 | 0.36 |
| ARG48 | H | 1.00 | 0.002 | 1.00 | -217643.00 |

3.47.11 Detailed Probabilities of PHE47HB3:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE47 | 0.88 | 1.00 |
| ARG48 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F47HA | 1.00 |
| F47HB2 | 1.00 |
| F47HD1 | 1.00 |
| F47HD2 | 1.00 |
| F47HE2 | 1.00 |
| F47H | 1.00 |
| F47HB3 | 1.00 |
| R48H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE47 | HA | 1.00 | 0.001 | 1.00 | 1.80 |
| PHE47 | HB2 | 1.00 | 0.007 | 1.00 | 5.38 |
| PHE47 | HB3 | 1.00 | 0.111 | 0.00 | 0.00 |
| PHE47 | HD1 | 1.00 | 0.004 | 1.00 | 0.85 |
| PHE47 | HD2 | 1.00 | 0.004 | 1.00 | 0.85 |
| PHE47 | HE2 | 1.00 | 0.001 | 1.00 | 0.11 |
| PHE47 | H | 1.00 | 0.004 | 1.00 | -1597845.00 |
| PHE47 | HE1 | 0.89 | 0.001 | 1.00 | 0.11 |
| ARG48 | H | 1.00 | 0.008 | 1.00 | -427671.00 |
| ARG48 | HA | 0.85 | 0.012 | 1.00 | 0.49 |

3.47.12 Detailed Probabilities of PHE47HD1:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE47 | 0.78 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F47HA | 1.00 |
| F47HB2 | 1.00 |
| F47HB3 | 1.00 |
| F47HD2 | 1.00 |
| F47HE1 | 1.00 |
| F47HE2 | 1.00 |
| F47HZ | 1.00 |
| F47H | 1.00 |
| F47HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE47 | HA | 1.00 | 0.024 | 1.00 | 0.75 |
| PHE47 | HB2 | 1.00 | 0.008 | 1.00 | 1.23 |
| PHE47 | HB3 | 1.00 | 0.012 | 1.00 | 1.20 |
| PHE47 | HD1 | 1.00 | 0.001 | 1.00 | 5.68 |
| PHE47 | HD2 | 1.00 | 0.001 | 1.00 | 5.68 |
| PHE47 | HE1 | 1.00 | 0.049 | 0.00 | 0.00 |
| PHE47 | HE2 | 1.00 | 0.049 | 0.00 | 0.00 |
| PHE47 | HZ | 1.00 | 0.012 | 1.00 | 20.18 |
| PHE47 | H | 1.00 | 0.030 | 1.00 | 0.00 |

3.47.13 Detailed Probabilities of PHE47HD2:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE47 | 0.78 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F47HA | 1.00 |
| F47HB2 | 1.00 |
| F47HB3 | 1.00 |
| F47HD1 | 1.00 |
| F47HE1 | 1.00 |
| F47HE2 | 1.00 |
| F47HZ | 1.00 |
| F47H | 0.99 |
| F47HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE47 | HA | 1.00 | 0.024 | 1.00 | 0.75 |
| PHE47 | HB2 | 1.00 | 0.008 | 1.00 | 1.23 |
| PHE47 | HB3 | 1.00 | 0.012 | 1.00 | 1.20 |
| PHE47 | HD1 | 1.00 | 0.001 | 1.00 | 5.68 |
| PHE47 | HD2 | 1.00 | 0.001 | 1.00 | 5.68 |
| PHE47 | HE1 | 1.00 | 0.049 | 0.00 | 0.00 |
| PHE47 | HE2 | 1.00 | 0.049 | 0.00 | 0.00 |
| PHE47 | HZ | 1.00 | 0.012 | 1.00 | 20.18 |
| PHE47 | H | 0.99 | 0.030 | 1.00 | 0.00 |

3.47.14 Detailed Probabilities of PHE47HE1:

Overall probability: 0.400

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE47 | 0.40 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F47HD1 | 1.00 |
| F47HD2 | 1.00 |
| F47HE2 | 1.00 |
| F47HZ | 1.00 |
| F47HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE47 | HD1 | 1.00 | 0.058 | 0.00 | 0.00 |
| PHE47 | HD2 | 1.00 | 0.058 | 0.00 | 0.00 |
| PHE47 | HE1 | 1.00 | 0.008 | 1.00 | 16.89 |
| PHE47 | HE2 | 1.00 | 0.008 | 1.00 | 16.89 |
| PHE47 | HZ | 1.00 | 0.044 | 0.00 | 0.00 |

3.47.15 Detailed Probabilities of PHE47HE2:

Overall probability: 0.286

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE47 | 0.29 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F47HB2 | 1.00 |
| F47HB3 | 1.00 |
| F47HD1 | 1.00 |
| F47HD2 | 1.00 |
| F47HE1 | 1.00 |
| F47HZ | 1.00 |
| F47HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE47 | HB2 | 1.00 | 0.051 | 0.00 | 0.00 |
| PHE47 | HB3 | 1.00 | 0.047 | 0.00 | 0.00 |
| PHE47 | HD1 | 1.00 | 0.058 | 0.00 | 0.00 |
| PHE47 | HD2 | 1.00 | 0.058 | 0.00 | 0.00 |
| PHE47 | HE1 | 1.00 | 0.008 | 1.00 | 16.89 |
| PHE47 | HE2 | 1.00 | 0.008 | 1.00 | 16.89 |
| PHE47 | HZ | 1.00 | 0.044 | 0.00 | 0.00 |

3.47.16 Detailed Probabilities of PHE47HZ:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE47 | 0.60 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F47HD1 | 1.00 |
| F47HD2 | 1.00 |
| F47HE1 | 1.00 |
| F47HE2 | 1.00 |
| F47HZ | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE47 | HD1 | 1.00 | 0.002 | 1.00 | 23.43 |
| PHE47 | HD2 | 1.00 | 0.002 | 1.00 | 23.43 |
| PHE47 | HE1 | 1.00 | 0.053 | 0.00 | 0.00 |
| PHE47 | HE2 | 1.00 | 0.053 | 0.00 | 0.00 |
| PHE47 | HZ | 1.00 | 0.016 | 1.00 | 20.18 |

3.47.17 Detailed Probabilities of PHE47H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA46 | 1.00 | 1.00 |
| PHE47 | 1.00 | 1.00 |
| ARG48 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A46HA | 1.00 |
| A46HB1 | 1.00 |
| A46H | 1.00 |
| F47HA | 1.00 |
| F47HB2 | 1.00 |
| F47HB3 | 1.00 |
| F47HD1 | 1.00 |
| F47HD2 | 0.99 |
| F47H | 1.00 |
| R48H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA46 | HA | 1.00 | 0.001 | 1.00 | 0.14 |
| ALA46 | HB1 | 1.00 | 0.005 | 1.00 | 0.22 |
| ALA46 | H | 1.00 | 0.004 | 1.00 | -1339206.00 |
| PHE47 | HA | 1.00 | 0.004 | 1.00 | 0.75 |
| PHE47 | HB2 | 1.00 | 0.020 | 1.00 | 1.23 |
| PHE47 | HB3 | 1.00 | 0.016 | 1.00 | 1.20 |
| PHE47 | HD1 | 1.00 | 0.027 | 1.00 | 5.68 |
| PHE47 | HD2 | 0.99 | 0.027 | 1.00 | 5.68 |
| PHE47 | H | 1.00 | 0.002 | 1.00 | -9285072.00 |
| ARG48 | H | 1.00 | 0.002 | 1.00 | -535145.00 |

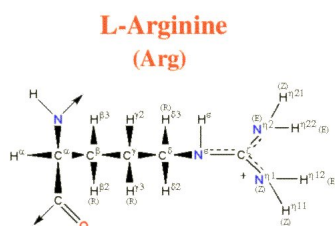


Figure 38: Image from the BMRB

Residue probability: 0.922
 Residue probability confidence: 0.867

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 174.898 | 176.453 | 2.303 | 0.000 | 0.000 |
| CA 3.48.1 | 55.899 | 56.803 | 3.326 | 0.742 | 1.000 |
| CB 3.48.2 | 30.330 | 30.892 | 2.424 | 1.000 | 0.889 |
| CG 3.48.3 | 26.984 | 27.247 | 1.538 | 1.000 | 0.800 |
| CD 3.48.4 | 43.100 | 43.189 | 1.415 | 0.861 | 0.667 |
| N 3.48.5 | 115.511 | 120.701 | 3.779 | 1.000 | 1.000 |
| NE | NA | - | - | 0.000 | 0.000 |
| NH1 | NA | - | - | 0.000 | 0.000 |
| NH2 | NA | - | - | 0.000 | 0.000 |
| HA 3.48.6 | 4.216 | 4.301 | 0.495 | 0.848 | 1.000 |
| HB2 3.48.7 | 1.941 | 1.793 | 0.292 | 1.000 | 0.889 |
| HB3 3.48.8 | 1.622 | 1.757 | 0.307 | 0.750 | 0.889 |
| HG2 3.48.9 | 1.235 | 1.559 | 0.294 | 0.925 | 0.800 |
| HG3 3.48.10 | 1.129 | 1.535 | 0.310 | 1.000 | 0.800 |
| HD 3.48.11 | 3.112 | 3.105 | 0.301 | 1.000 | 0.667 |
| H 3.48.12 | 6.985 | 8.248 | 0.623 | 0.938 | 1.000 |
| HE | NA | - | - | 0.000 | 0.000 |
| HH1 | NA | - | - | 0.000 | 0.000 |
| HH2 | NA | - | - | 0.000 | 0.000 |

3.48.1 Detailed Probabilities of ARG48CA:

Overall probability: 0.742
 Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE47 | 0.63 | 1.00 |
| ARG48 | 0.71 | 1.00 |
| SER49 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F47HA | 1.00 |
| R48HB2 | 1.00 |
| R48HB3 | 1.00 |
| R48HG2 | 1.00 |
| R48HG3 | 1.00 |
| R48HD2 | 0.98 |
| R48H | 1.00 |
| R48HA | 1.00 |
| S49HA | 1.00 |
| S49H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE47 | HA | 1.00 | 0.214 | 0.00 | 0.00 |
| PHE47 | HB3 | 0.85 | 0.012 | 1.00 | 0.49 |
| PHE47 | H | 0.90 | 0.032 | 0.90 | 0.00 |
| ARG48 | HA | 1.00 | 0.209 | 0.00 | 0.00 |
| ARG48 | HB2 | 1.00 | 0.004 | 1.00 | 1.02 |
| ARG48 | HB3 | 1.00 | 0.275 | 0.00 | 0.00 |
| ARG48 | HG2 | 1.00 | 0.007 | 1.00 | 0.70 |
| ARG48 | HG3 | 1.00 | 0.010 | 1.00 | 0.28 |
| ARG48 | HD2 | 0.98 | 0.002 | 1.00 | 0.49 |
| ARG48 | H | 1.00 | 0.005 | 1.00 | 0.35 |
| SER49 | HA | 1.00 | 0.013 | 1.00 | 0.06 |
| SER49 | H | 1.00 | 0.008 | 1.00 | 0.29 |

3.48.2 Detailed Probabilities of ARG48CB:

Overall probability: 1.000

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG48 | 1.00 | 0.88 |
| SER49 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R48HA | 1.00 |
| R48HB3 | 1.00 |
| R48HG2 | 1.00 |
| R48HG3 | 1.00 |
| R48HD2 | 1.00 |
| R48H | 1.00 |
| R48HE | 1.00 |
| R48HB2 | 1.00 |
| S49H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG48 | HA | 1.00 | 0.003 | 1.00 | 1.00 |
| ARG48 | HB2 | 1.00 | 0.009 | 1.00 | 29.96 |
| ARG48 | HB3 | 1.00 | 0.003 | 1.00 | 3.85 |
| ARG48 | HG2 | 1.00 | 0.002 | 1.00 | 0.86 |
| ARG48 | HG3 | 1.00 | 0.010 | 1.00 | 0.54 |
| ARG48 | HD2 | 1.00 | 0.001 | 1.00 | 0.86 |
| ARG48 | H | 1.00 | 0.006 | 1.00 | 0.27 |
| SER49 | H | 1.00 | 0.011 | 1.00 | 0.14 |

3.48.3 Detailed Probabilities of ARG48CG:

Overall probability: 1.000

Overall confidence: 0.800

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG48 | 1.00 | 0.78 |
| SER49 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R48HA | 1.00 |
| R48HB2 | 1.00 |
| R48HB3 | 1.00 |
| R48HG3 | 1.00 |
| R48HD2 | 1.00 |
| R48H | 1.00 |
| R48HE | 1.00 |
| R48HH11 | 1.00 |
| R48HG2 | 1.00 |
| S49H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG48 | HA | 1.00 | 0.002 | 1.00 | 0.39 |
| ARG48 | HB2 | 1.00 | 0.014 | 1.00 | 1.71 |
| ARG48 | HB3 | 1.00 | 0.004 | 1.00 | 0.48 |
| ARG48 | HG2 | 1.00 | 0.001 | 1.00 | 10.96 |
| ARG48 | HG3 | 1.00 | 0.005 | 1.00 | 3.50 |
| ARG48 | HD2 | 1.00 | 0.001 | 1.00 | 0.91 |
| ARG48 | H | 1.00 | 0.008 | 1.00 | 0.23 |
| SER49 | H | 0.97 | 0.016 | 1.00 | 0.07 |

3.48.4 Detailed Probabilities of ARG48CD:

Overall probability: 0.861

Overall confidence: 0.667

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG48 | 0.86 | 0.67 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R48HA | 0.98 |
| R48HB2 | 1.00 |
| R48HB3 | 1.00 |
| R48HG2 | 1.00 |
| R48HG3 | 1.00 |
| R48HD3 | 1.00 |
| R48HE | 1.00 |
| R48HH11 | 1.00 |
| R48HH21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG48 | HA | 0.97 | 0.104 | 0.03 | 0.00 |
| ARG48 | HB2 | 1.00 | 0.001 | 1.00 | 1.07 |
| ARG48 | HB3 | 1.00 | 0.003 | 1.00 | 0.99 |
| ARG48 | HG2 | 1.00 | 0.006 | 1.00 | 1.69 |
| ARG48 | HG3 | 1.00 | 0.002 | 1.00 | 1.59 |
| ARG48 | HD2 | 1.00 | 0.002 | 1.00 | 61.85 |
| ARG48 | H | 0.86 | 0.001 | 1.00 | 0.13 |

3.48.5 Detailed Probabilities of ARG48N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE47 | 1.00 | 1.00 |
| ARG48 | 1.00 | 1.00 |
| SER49 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F47HB2 | 1.00 |
| F47H | 1.00 |
| F47HA | 1.00 |
| F47HB3 | 1.00 |
| R48HA | 1.00 |
| R48HB2 | 1.00 |
| R48HB3 | 1.00 |
| R48HG2 | 1.00 |
| R48HG3 | 1.00 |
| R48H | 1.00 |
| S49H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE47 | HA | 1.00 | 0.004 | 1.00 | -967450.00 |
| PHE47 | HB2 | 1.00 | 0.002 | 1.00 | -217643.00 |
| PHE47 | HB3 | 1.00 | 0.008 | 1.00 | -427671.00 |
| PHE47 | H | 1.00 | 0.002 | 1.00 | -535145.00 |
| PHE47 | HD1 | 0.73 | 0.026 | 1.00 | -535145.00 |
| PHE47 | HD2 | 0.68 | 0.026 | 1.00 | -535145.00 |
| ARG48 | HA | 1.00 | 0.002 | 1.00 | -967450.00 |
| ARG48 | HB2 | 1.00 | 0.005 | 1.00 | -577494.00 |
| ARG48 | HB3 | 1.00 | 0.006 | 1.00 | -839784.00 |
| ARG48 | HG2 | 1.00 | 0.000 | 1.00 | -628228.00 |
| ARG48 | HG3 | 1.00 | 0.001 | 1.00 | -692922.00 |
| ARG48 | H | 1.00 | 0.000 | 1.00 | -5690033.00 |
| ARG48 | HD2 | 0.87 | 0.002 | 1.00 | -427671.00 |
| SER49 | H | 1.00 | 0.004 | 1.00 | -970521.00 |
| SER49 | HB2 | 0.54 | 0.002 | 1.00 | -217643.00 |

3.48.6 Detailed Probabilities of ARG48HA:

Overall probability: 0.848

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE47 | 1.00 | 1.00 |
| ARG48 | 0.72 | 1.00 |
| SER49 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F47HA | 1.00 |
| R48HB2 | 1.00 |
| R48HB3 | 1.00 |
| R48HG2 | 1.00 |
| R48HG3 | 1.00 |
| R48HD2 | 0.98 |
| R48H | 1.00 |
| R48HA | 1.00 |
| S49HA | 1.00 |
| S49H | 1.00 |

NOESY contacts detailed probability

3.48 ARG(48)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE47 | HA | 1.00 | 0.010 | 1.00 | 10.19 |
| PHE47 | HB2 | 0.64 | 0.010 | 1.00 | 1.41 |
| PHE47 | HB3 | 0.85 | 0.010 | 1.00 | 1.26 |
| PHE47 | H | 0.90 | 0.010 | 1.00 | -1103594.00 |
| ARG48 | HA | 1.00 | 0.209 | 0.00 | 0.00 |
| ARG48 | HB2 | 1.00 | 0.003 | 1.00 | 1.00 |
| ARG48 | HB3 | 1.00 | 0.001 | 1.00 | 0.63 |
| ARG48 | HG2 | 1.00 | 0.002 | 1.00 | 0.39 |
| ARG48 | HG3 | 1.00 | 0.002 | 1.00 | 0.26 |
| ARG48 | HD2 | 0.98 | 0.104 | 0.02 | 0.00 |
| ARG48 | H | 1.00 | 0.002 | 1.00 | -967450.00 |
| SER49 | HA | 1.00 | 0.014 | 1.00 | 0.05 |
| SER49 | H | 1.00 | 0.004 | 1.00 | -823461.00 |

3.48.7 Detailed Probabilities of ARG48HB2:

Overall probability: 1.000

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG48 | 1.00 | 0.88 |
| SER49 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R48HA | 1.00 |
| R48HB3 | 1.00 |
| R48HG2 | 1.00 |
| R48HG3 | 1.00 |
| R48HD2 | 1.00 |
| R48H | 1.00 |
| R48HE | 1.00 |
| R48HB2 | 1.00 |
| S49H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG48 | HA | 1.00 | 0.004 | 1.00 | 1.02 |
| ARG48 | HB2 | 1.00 | 0.009 | 1.00 | 29.96 |
| ARG48 | HB3 | 1.00 | 0.002 | 1.00 | 3.51 |
| ARG48 | HG2 | 1.00 | 0.014 | 1.00 | 1.71 |
| ARG48 | HG3 | 1.00 | 0.004 | 1.00 | 0.38 |
| ARG48 | HD2 | 1.00 | 0.001 | 1.00 | 1.07 |
| ARG48 | H | 1.00 | 0.005 | 1.00 | -577494.00 |
| SER49 | H | 1.00 | 0.006 | 1.00 | -281691.00 |

3.48.8 Detailed Probabilities of ARG48HB3:

Overall probability: 0.750

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG48 | 0.71 | 0.88 |
| SER49 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R48HA | 1.00 |
| R48HB2 | 1.00 |
| R48HG2 | 1.00 |
| R48HG3 | 1.00 |
| R48HD2 | 1.00 |
| R48H | 1.00 |
| R48HE | 1.00 |
| R48HB3 | 1.00 |
| S49H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG48 | HA | 1.00 | 0.275 | 0.00 | 0.00 |
| ARG48 | HB2 | 1.00 | 0.003 | 1.00 | 3.85 |
| ARG48 | HB3 | 1.00 | 0.317 | 0.00 | 0.00 |
| ARG48 | HG2 | 1.00 | 0.004 | 1.00 | 0.48 |
| ARG48 | HG3 | 1.00 | 0.010 | 1.00 | 0.38 |
| ARG48 | HD2 | 1.00 | 0.003 | 1.00 | 0.99 |
| ARG48 | H | 1.00 | 0.006 | 1.00 | -839784.00 |
| SER49 | H | 1.00 | 0.009 | 1.00 | -230656.00 |

3.48.9 Detailed Probabilities of ARG48HG2:

Overall probability: 0.925

Overall confidence: 0.800

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG48 | 1.00 | 0.78 |
| SER49 | 0.40 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R48HA | 1.00 |
| R48HB2 | 1.00 |
| R48HB3 | 1.00 |
| R48HG3 | 1.00 |
| R48HD2 | 1.00 |
| R48H | 1.00 |
| R48HE | 1.00 |
| R48HH11 | 1.00 |
| R48HG2 | 1.00 |
| S49H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG48 | HA | 1.00 | 0.007 | 1.00 | 0.70 |
| ARG48 | HB2 | 1.00 | 0.002 | 1.00 | 0.86 |
| ARG48 | HB3 | 1.00 | 0.000 | 1.00 | 0.49 |
| ARG48 | HG2 | 1.00 | 0.001 | 1.00 | 10.96 |
| ARG48 | HG3 | 1.00 | 0.006 | 1.00 | 3.14 |
| ARG48 | HD2 | 1.00 | 0.006 | 1.00 | 1.69 |
| ARG48 | H | 1.00 | 0.000 | 1.00 | -628228.00 |
| SER49 | H | 0.97 | 0.036 | 0.40 | 0.00 |

3.48.10 Detailed Probabilities of ARG48HG3:

Overall probability: 1.000

Overall confidence: 0.800

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG48 | 1.00 | 0.78 |
| SER49 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R48HA | 1.00 |
| R48HB2 | 1.00 |
| R48HB3 | 1.00 |
| R48HG2 | 1.00 |
| R48HD2 | 1.00 |
| R48H | 1.00 |
| R48HE | 1.00 |
| R48HH11 | 1.00 |
| R48HG3 | 1.00 |
| S49H | 0.96 |

NOESY contacts detailed probability

3.48 ARG(48)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG48 | HA | 1.00 | 0.010 | 1.00 | 0.28 |
| ARG48 | HB2 | 1.00 | 0.010 | 1.00 | 0.54 |
| ARG48 | HB3 | 1.00 | 0.001 | 1.00 | 0.53 |
| ARG48 | HG2 | 1.00 | 0.005 | 1.00 | 3.50 |
| ARG48 | HG3 | 1.00 | 0.003 | 1.00 | 5.13 |
| ARG48 | HD2 | 1.00 | 0.002 | 1.00 | 1.59 |
| ARG48 | H | 1.00 | 0.001 | 1.00 | -692922.00 |
| SER49 | H | 0.96 | 0.020 | 1.00 | -105114.00 |

3.48.11 Detailed Probabilities of ARG48HD2:

Overall probability: 1.000

Overall confidence: 0.667

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG48 | 1.00 | 0.67 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R48HA | 0.98 |
| R48HB2 | 1.00 |
| R48HB3 | 1.00 |
| R48HG2 | 1.00 |
| R48HG3 | 1.00 |
| R48HD3 | 1.00 |
| R48HE | 1.00 |
| R48HH11 | 1.00 |
| R48HH21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG48 | HA | 0.97 | 0.002 | 1.00 | 0.49 |
| ARG48 | HB2 | 1.00 | 0.001 | 1.00 | 0.86 |
| ARG48 | HB3 | 1.00 | 0.003 | 1.00 | 0.64 |
| ARG48 | HG2 | 1.00 | 0.001 | 1.00 | 0.91 |
| ARG48 | HG3 | 1.00 | 0.002 | 1.00 | 0.79 |
| ARG48 | HD2 | 1.00 | 0.002 | 1.00 | 61.85 |
| ARG48 | H | 0.86 | 0.002 | 1.00 | -427671.00 |

3.48.12 Detailed Probabilities of ARG48H:

Overall probability: 0.938

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE47 | 0.83 | 1.00 |
| ARG48 | 1.00 | 1.00 |
| SER49 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F47HB2 | 1.00 |
| F47H | 1.00 |
| F47HA | 1.00 |
| F47HB3 | 1.00 |
| R48HA | 1.00 |
| R48HB2 | 1.00 |
| R48HB3 | 1.00 |
| R48HG2 | 1.00 |
| R48HG3 | 1.00 |
| R48H | 1.00 |
| S49H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE47 | HA | 1.00 | 0.012 | 1.00 | 0.15 |
| PHE47 | HB2 | 1.00 | 0.009 | 1.00 | 0.11 |
| PHE47 | HB3 | 1.00 | 0.345 | 0.00 | 0.00 |
| PHE47 | H | 1.00 | 0.002 | 1.00 | -460786.00 |
| PHE47 | HD1 | 0.73 | 0.011 | 1.00 | 0.33 |
| PHE47 | HD2 | 0.68 | 0.011 | 1.00 | 0.33 |
| ARG48 | HA | 1.00 | 0.005 | 1.00 | 0.35 |
| ARG48 | HB2 | 1.00 | 0.006 | 1.00 | 0.27 |
| ARG48 | HB3 | 1.00 | 0.000 | 1.00 | 0.32 |
| ARG48 | HG2 | 1.00 | 0.008 | 1.00 | 0.23 |
| ARG48 | HG3 | 1.00 | 0.002 | 1.00 | 0.19 |
| ARG48 | H | 1.00 | 0.000 | 1.00 | -5690033.00 |
| ARG48 | HD2 | 0.87 | 0.001 | 1.00 | 0.13 |
| SER49 | H | 1.00 | 0.002 | 1.00 | -941762.00 |
| SER49 | HA | 0.87 | 0.026 | 1.00 | 0.14 |
| SER49 | HB2 | 0.54 | 0.023 | 1.00 | 0.09 |

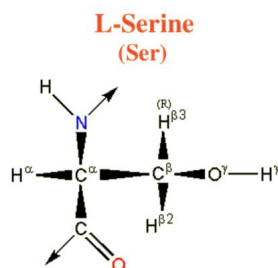
3.49 SER(49)

Figure 39: Image from the BMRB

Residue probability: 0.852

Residue probability confidence: 0.885

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | NA | – | – | 0.000 | 0.000 |
| CA 3.49.1 | 53.401 | 58.750 | 3.025 | 1.000 | 0.889 |
| CB 3.49.2 | 65.466 | 63.523 | 4.288 | 0.836 | 0.857 |
| N 3.49.3 | 111.050 | 116.135 | 5.326 | 0.929 | 0.923 |
| HA 3.49.4 | 5.524 | 4.486 | 0.430 | 0.909 | 0.889 |
| HB2 3.49.5 | 3.230 | 3.856 | 0.325 | 0.510 | 0.857 |
| HB3 3.49.6 | 3.823 | 3.825 | 0.343 | 0.857 | 0.857 |
| H 3.49.7 | 7.711 | 8.292 | 0.600 | 0.920 | 0.923 |
| HG | NA | – | – | 0.000 | 0.000 |

3.49.1 Detailed Probabilities of SER49CA:

Overall probability: 1.000

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG48 | 1.00 | 1.00 |
| SER49 | 1.00 | 0.80 |
| PRO50 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R48HA | 1.00 |
| S49HB2 | 1.00 |
| S49HB3 | 1.00 |
| S49H | 1.00 |
| S49HG | 1.00 |
| S49HA | 1.00 |
| P50HA | 1.00 |
| P50HD3 | 1.00 |
| P50HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG48 | HA | 1.00 | 0.014 | 1.00 | 0.05 |
| ARG48 | H | 0.87 | 0.026 | 1.00 | 0.14 |
| SER49 | HA | 1.00 | 0.012 | 1.00 | 3.13 |
| SER49 | HB2 | 1.00 | 0.015 | 1.00 | 0.46 |
| SER49 | HB3 | 1.00 | 0.026 | 1.00 | 0.70 |
| SER49 | H | 1.00 | 0.007 | 1.00 | 0.15 |
| PRO50 | HA | 1.00 | 0.008 | 1.00 | 0.05 |
| PRO50 | HD2 | 1.00 | 0.009 | 1.00 | 0.53 |
| PRO50 | HD3 | 1.00 | 0.014 | 1.00 | 0.70 |
| PRO50 | HG2 | 0.94 | 0.002 | 1.00 | 0.10 |
| PRO50 | HG3 | 0.89 | 0.019 | 1.00 | 0.12 |

3.49.2 Detailed Probabilities of SER49CB:

Overall probability: 0.836

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER49 | 1.00 | 0.80 |
| PRO50 | 0.51 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S49HA | 1.00 |
| S49HB2 | 1.00 |
| S49H | 1.00 |
| S49HG | 1.00 |
| S49HB3 | 1.00 |
| P50HD3 | 0.99 |
| P50HD2 | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER49 | HA | 1.00 | 0.004 | 1.00 | 0.34 |
| SER49 | HB2 | 1.00 | 0.002 | 1.00 | 1.09 |
| SER49 | HB3 | 1.00 | 0.017 | 1.00 | 26.96 |
| SER49 | H | 1.00 | 0.000 | 1.00 | 0.22 |
| PRO50 | HD2 | 0.97 | 0.009 | 1.00 | 0.14 |
| PRO50 | HD3 | 0.99 | 0.057 | 0.01 | 0.00 |

3.49.3 Detailed Probabilities of SER49N:

Overall probability: 0.929

Overall confidence: 0.923

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG48 | 0.91 | 1.00 |
| SER49 | 1.00 | 0.80 |
| PRO50 | 0.87 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R48HB3 | 1.00 |
| R48HB2 | 1.00 |
| R48HA | 1.00 |
| R48HG3 | 0.96 |
| R48HG2 | 0.97 |
| R48H | 1.00 |
| S49HA | 1.00 |
| S49HB2 | 1.00 |
| S49HB3 | 1.00 |
| S49HG | 1.00 |
| S49H | 1.00 |
| P50HD3 | 0.96 |
| P50HD2 | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG48 | HA | 1.00 | 0.004 | 1.00 | -823461.00 |
| ARG48 | HB2 | 1.00 | 0.006 | 1.00 | -281691.00 |
| ARG48 | HB3 | 1.00 | 0.009 | 1.00 | -230656.00 |
| ARG48 | HG2 | 0.97 | 0.036 | 0.40 | 0.00 |
| ARG48 | HG3 | 0.96 | 0.020 | 1.00 | -105114.00 |
| ARG48 | H | 1.00 | 0.002 | 1.00 | -941762.00 |
| ARG48 | HD2 | 0.55 | 0.001 | 1.00 | -241980.00 |
| SER49 | HA | 1.00 | 0.003 | 1.00 | -662645.00 |
| SER49 | HB2 | 1.00 | 0.006 | 1.00 | -1064123.00 |
| SER49 | HB3 | 1.00 | 0.006 | 1.00 | -832016.00 |
| SER49 | H | 1.00 | 0.004 | 1.00 | -16088325.00 |
| PRO50 | HD2 | 0.98 | 0.013 | 1.00 | -204631.00 |
| PRO50 | HD3 | 0.96 | 0.034 | 0.60 | 0.00 |
| PRO50 | HA | 0.65 | 0.018 | 1.00 | -823461.00 |

3.49.4 Detailed Probabilities of SER49HA:

Overall probability: 0.909

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG48 | 1.00 | 1.00 |
| SER49 | 1.00 | 0.80 |
| PRO50 | 0.83 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R48HA | 1.00 |
| S49HB2 | 1.00 |
| S49HB3 | 1.00 |
| S49H | 1.00 |
| S49HG | 1.00 |
| S49HA | 1.00 |
| P50HA | 1.00 |
| P50HD3 | 1.00 |
| P50HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG48 | HA | 1.00 | 0.013 | 1.00 | 0.06 |
| SER49 | HA | 1.00 | 0.012 | 1.00 | 3.13 |
| SER49 | HB2 | 1.00 | 0.003 | 1.00 | 0.20 |
| SER49 | HB3 | 1.00 | 0.004 | 1.00 | 0.34 |
| SER49 | H | 1.00 | 0.003 | 1.00 | -662645.00 |
| PRO50 | HA | 1.00 | 0.340 | 0.00 | 0.00 |
| PRO50 | HD2 | 1.00 | 0.003 | 1.00 | 0.56 |
| PRO50 | HD3 | 1.00 | 0.003 | 1.00 | 0.62 |
| PRO50 | HB3 | 0.78 | 0.013 | 1.00 | 0.06 |
| PRO50 | HG2 | 0.94 | 0.000 | 1.00 | 0.16 |
| PRO50 | HG3 | 0.89 | 0.003 | 1.00 | 0.14 |

3.49.5 Detailed Probabilities of SER49HB2:

Overall probability: 0.510

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER49 | 0.75 | 0.80 |
| PRO50 | 0.03 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S49HA | 1.00 |
| S49HB3 | 1.00 |
| S49H | 1.00 |
| S49HG | 1.00 |
| S49HB2 | 1.00 |
| P50HD3 | 0.98 |
| P50HD2 | 0.96 |

NOESY contacts detailed probability

3.49 SER(49)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER49 | HA | 1.00 | 0.015 | 1.00 | 0.46 |
| SER49 | HB2 | 1.00 | 0.591 | 0.00 | 0.00 |
| SER49 | HB3 | 1.00 | 0.002 | 1.00 | 1.09 |
| SER49 | H | 1.00 | 0.006 | 1.00 | -1064123.00 |
| PRO50 | HD2 | 0.96 | 0.319 | 0.04 | 0.00 |
| PRO50 | HD3 | 0.98 | 0.388 | 0.02 | 0.00 |

3.49.6 Detailed Probabilities of SER49HB3:

Overall probability: 0.857

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER49 | 1.00 | 0.80 |
| PRO50 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S49HA | 1.00 |
| S49HB2 | 1.00 |
| S49H | 1.00 |
| S49HG | 1.00 |
| S49HB3 | 1.00 |
| P50HD3 | 0.99 |
| P50HD2 | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER49 | HA | 1.00 | 0.026 | 1.00 | 0.70 |
| SER49 | HB2 | 1.00 | 0.002 | 1.00 | 1.04 |
| SER49 | HB3 | 1.00 | 0.017 | 1.00 | 26.96 |
| SER49 | H | 1.00 | 0.006 | 1.00 | -832016.00 |
| PRO50 | HD2 | 0.97 | 0.036 | 0.40 | 0.00 |
| PRO50 | HD3 | 0.99 | 0.034 | 0.60 | 0.00 |
| PRO50 | HA | 0.72 | 0.023 | 1.00 | 0.23 |

3.49.7 Detailed Probabilities of SER49H:

Overall probability: 0.920

Overall confidence: 0.923

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG48 | 0.84 | 1.00 |
| SER49 | 1.00 | 0.80 |
| PRO50 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R48HB3 | 1.00 |
| R48HB2 | 1.00 |
| R48HA | 1.00 |
| R48HG3 | 0.96 |
| R48HG2 | 0.97 |
| R48H | 1.00 |
| S49HA | 1.00 |
| S49HB2 | 1.00 |
| S49HB3 | 1.00 |
| S49HG | 1.00 |
| S49H | 1.00 |
| P50HD3 | 0.96 |
| P50HD2 | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG48 | HA | 1.00 | 0.008 | 1.00 | 0.29 |
| ARG48 | HB2 | 1.00 | 0.011 | 1.00 | 0.14 |
| ARG48 | HB3 | 1.00 | 0.010 | 1.00 | 0.12 |
| ARG48 | HG2 | 0.97 | 0.016 | 1.00 | 0.07 |
| ARG48 | HG3 | 0.96 | 0.364 | 0.04 | 0.00 |
| ARG48 | H | 1.00 | 0.004 | 1.00 | -970521.00 |
| SER49 | HA | 1.00 | 0.007 | 1.00 | 0.15 |
| SER49 | HB2 | 1.00 | 0.002 | 1.00 | 0.20 |
| SER49 | HB3 | 1.00 | 0.000 | 1.00 | 0.22 |
| SER49 | H | 1.00 | 0.004 | 1.00 | -16088325.00 |
| PRO50 | HD2 | 0.98 | 0.011 | 1.00 | 0.07 |
| PRO50 | HD3 | 0.96 | 0.011 | 1.00 | 0.06 |

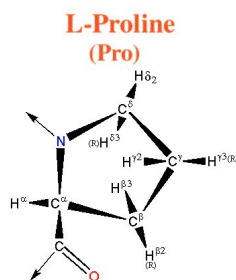


Figure 40: Image from the BMRB

Residue probability: 0.780
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 178.097 | 175.173 | 13.901 | 0.000 | 0.000 |
| CA 3.50.1 | 64.757 | 62.931 | 15.301 | 0.873 | 1.000 |
| CB 3.50.2 | 32.122 | 33.632 | 13.629 | 0.750 | 1.000 |
| CG 3.50.3 | 27.711 | 28.412 | 13.801 | 0.871 | 1.000 |
| CD 3.50.4 | 50.987 | 49.797 | 3.175 | 0.713 | 1.000 |
| N | NA | - | - | 0.000 | 0.000 |
| HA 3.50.5 | 4.194 | 4.332 | 0.427 | 0.818 | 1.000 |
| HB2 3.50.6 | 2.051 | 2.099 | 0.501 | 0.778 | 1.000 |
| HB3 3.50.7 | 2.549 | 2.052 | 0.596 | 0.750 | 1.000 |
| HG2 3.50.8 | 2.293 | 1.927 | 0.364 | 1.000 | 1.000 |
| HG3 3.50.9 | 2.101 | 1.907 | 0.417 | 0.514 | 1.000 |
| HD2 3.50.10 | 3.970 | 3.640 | 0.682 | 0.822 | 1.000 |
| HD3 3.50.11 | 3.863 | 3.558 | 0.522 | 0.694 | 1.000 |

3.50.1 Detailed Probabilities of PRO50CA:

Overall probability: 0.873
Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER49 | 0.50 | 1.00 |
| PRO50 | 0.94 | 1.00 |
| LEU51 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S49HA | 1.00 |
| P50HB2 | 1.00 |
| P50HB3 | 1.00 |
| P50HG2 | 1.00 |
| P50HG3 | 1.00 |
| P50HD2 | 1.00 |
| P50HD3 | 1.00 |
| P50HA | 1.00 |
| L51H | 1.00 |
| L51HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER49 | HA | 1.00 | 0.340 | 0.00 | 0.00 |
| SER49 | HB3 | 0.72 | 0.023 | 1.00 | 0.23 |
| PRO50 | HA | 1.00 | 0.003 | 1.00 | 8.81 |
| PRO50 | HB2 | 1.00 | 0.016 | 1.00 | 1.04 |
| PRO50 | HB3 | 1.00 | 0.000 | 1.00 | 1.62 |
| PRO50 | HG2 | 1.00 | 0.004 | 1.00 | 0.26 |
| PRO50 | HG3 | 1.00 | 0.034 | 0.60 | 0.00 |
| PRO50 | HD2 | 1.00 | 0.008 | 1.00 | 0.18 |
| PRO50 | HD3 | 1.00 | 0.017 | 1.00 | 0.23 |
| LEU51 | HA | 1.00 | 0.008 | 1.00 | 0.09 |
| LEU51 | H | 1.00 | 0.000 | 1.00 | 0.20 |

3.50.2 Detailed Probabilities of PRO50CB:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO50 | 0.71 | 1.00 |
| LEU51 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P50HA | 1.00 |
| P50HB2 | 1.00 |
| P50HG2 | 1.00 |
| P50HG3 | 1.00 |
| P50HD2 | 1.00 |
| P50HD3 | 1.00 |
| P50HB3 | 1.00 |
| L51H | 1.00 |

NOESY contacts detailed probability

3.50 PRO(50)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO50 | HA | 1.00 | 0.004 | 1.00 | 1.38 |
| PRO50 | HB2 | 1.00 | 0.001 | 1.00 | 3.95 |
| PRO50 | HB3 | 1.00 | 0.013 | 1.00 | 6.65 |
| PRO50 | HG2 | 1.00 | 0.001 | 1.00 | 0.91 |
| PRO50 | HG3 | 1.00 | 0.049 | 0.00 | 0.00 |
| PRO50 | HD2 | 1.00 | 0.114 | 0.00 | 0.00 |
| PRO50 | HD3 | 1.00 | 0.007 | 1.00 | 0.22 |
| LEU51 | H | 1.00 | 0.003 | 1.00 | 0.18 |

3.50.3 Detailed Probabilities of PRO50CG:

Overall probability: 0.871

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO50 | 0.87 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P50HA | 1.00 |
| P50HB2 | 1.00 |
| P50HB3 | 1.00 |
| P50HG3 | 1.00 |
| P50HD2 | 1.00 |
| P50HD3 | 1.00 |
| P50HG2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO50 | HA | 1.00 | 0.007 | 1.00 | 0.29 |
| PRO50 | HB2 | 1.00 | 0.039 | 0.10 | 0.00 |
| PRO50 | HB3 | 1.00 | 0.002 | 1.00 | 0.82 |
| PRO50 | HG2 | 1.00 | 0.002 | 1.00 | 6.41 |
| PRO50 | HG3 | 1.00 | 0.011 | 1.00 | 4.32 |
| PRO50 | HD2 | 1.00 | 0.000 | 1.00 | 0.80 |
| PRO50 | HD3 | 1.00 | 0.006 | 1.00 | 0.70 |

3.50.4 Detailed Probabilities of PRO50CD:

Overall probability: 0.713

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER49 | 0.61 | 1.00 |
| PRO50 | 0.77 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S49HA | 1.00 |
| S49H | 0.98 |
| S49HB3 | 0.97 |
| S49HB2 | 0.96 |
| P50HA | 1.00 |
| P50HB2 | 1.00 |
| P50HB3 | 1.00 |
| P50HG2 | 1.00 |
| P50HG3 | 1.00 |
| P50HD3 | 1.00 |
| P50HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER49 | HA | 1.00 | 0.003 | 1.00 | 0.56 |
| SER49 | HB2 | 0.96 | 0.319 | 0.04 | 0.00 |
| SER49 | HB3 | 0.97 | 0.036 | 0.40 | 0.00 |
| SER49 | H | 0.98 | 0.011 | 1.00 | 0.07 |
| PRO50 | HA | 1.00 | 0.003 | 1.00 | 0.14 |
| PRO50 | HB2 | 1.00 | 0.036 | 0.40 | 0.00 |
| PRO50 | HB3 | 1.00 | 0.060 | 0.00 | 0.00 |
| PRO50 | HG2 | 1.00 | 0.000 | 1.00 | 0.42 |
| PRO50 | HG3 | 1.00 | 0.000 | 1.00 | 1.16 |
| PRO50 | HD2 | 1.00 | 0.013 | 1.00 | 8.06 |
| PRO50 | HD3 | 1.00 | 0.004 | 1.00 | 1.62 |

3.50.5 Detailed Probabilities of PRO50HA:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER49 | 1.00 | 1.00 |
| PRO50 | 0.86 | 1.00 |
| LEU51 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S49HA | 1.00 |
| P50HB2 | 1.00 |
| P50HB3 | 1.00 |
| P50HG2 | 1.00 |
| P50HG3 | 1.00 |
| P50HD2 | 1.00 |
| P50HD3 | 1.00 |
| P50HA | 1.00 |
| L51H | 1.00 |
| L51HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER49 | HA | 1.00 | 0.008 | 1.00 | 0.05 |
| SER49 | H | 0.65 | 0.018 | 1.00 | -823461.00 |
| PRO50 | HA | 1.00 | 0.003 | 1.00 | 8.81 |
| PRO50 | HB2 | 1.00 | 0.008 | 1.00 | 0.63 |
| PRO50 | HB3 | 1.00 | 0.004 | 1.00 | 1.38 |
| PRO50 | HG2 | 1.00 | 0.007 | 1.00 | 0.29 |
| PRO50 | HG3 | 1.00 | 0.003 | 1.00 | 0.69 |
| PRO50 | HD2 | 1.00 | 0.003 | 1.00 | 0.14 |
| PRO50 | HD3 | 1.00 | 0.061 | 0.00 | 0.00 |
| LEU51 | HA | 1.00 | 0.191 | 0.00 | 0.00 |
| LEU51 | H | 1.00 | 0.003 | 1.00 | -268312.00 |

3.50.6 Detailed Probabilities of PRO50HB2:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO50 | 0.71 | 1.00 |
| LEU51 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P50HA | 1.00 |
| P50HB3 | 1.00 |
| P50HG2 | 1.00 |
| P50HG3 | 1.00 |
| P50HD2 | 1.00 |
| P50HD3 | 1.00 |
| P50HB2 | 1.00 |
| L51HA | 0.99 |
| L51H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO50 | HA | 1.00 | 0.016 | 1.00 | 1.04 |
| PRO50 | HB2 | 1.00 | 0.033 | 0.70 | 0.00 |
| PRO50 | HB3 | 1.00 | 0.001 | 1.00 | 3.95 |
| PRO50 | HG2 | 1.00 | 0.039 | 0.10 | 0.00 |
| PRO50 | HG3 | 1.00 | 0.032 | 0.80 | 0.00 |
| PRO50 | HD2 | 1.00 | 0.036 | 0.40 | 0.00 |
| PRO50 | HD3 | 1.00 | 0.004 | 1.00 | 0.64 |
| LEU51 | HA | 0.99 | 0.023 | 1.00 | 0.51 |
| LEU51 | H | 1.00 | 0.009 | 1.00 | -650405.00 |

3.50.7 Detailed Probabilities of PRO50HB3:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO50 | 0.71 | 1.00 |
| LEU51 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P50HA | 1.00 |
| P50HB2 | 1.00 |
| P50HG2 | 1.00 |
| P50HG3 | 1.00 |
| P50HD2 | 1.00 |
| P50HD3 | 1.00 |
| P50HB3 | 1.00 |
| L51H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO50 | HA | 1.00 | 0.000 | 1.00 | 1.62 |
| PRO50 | HB2 | 1.00 | 0.059 | 0.00 | 0.00 |
| PRO50 | HB3 | 1.00 | 0.013 | 1.00 | 6.65 |
| PRO50 | HG2 | 1.00 | 0.002 | 1.00 | 0.82 |
| PRO50 | HG3 | 1.00 | 0.001 | 1.00 | 0.91 |
| PRO50 | HD2 | 1.00 | 0.060 | 0.00 | 0.00 |
| PRO50 | HD3 | 1.00 | 0.003 | 1.00 | 0.12 |
| LEU51 | H | 1.00 | 0.001 | 1.00 | -255925.00 |

3.50.8 Detailed Probabilities of PRO50HG2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO50 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P50HA | 1.00 |
| P50HB2 | 1.00 |
| P50HB3 | 1.00 |
| P50HG3 | 1.00 |
| P50HD2 | 1.00 |
| P50HD3 | 1.00 |
| P50HG2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO50 | HA | 1.00 | 0.004 | 1.00 | 0.26 |
| PRO50 | HB2 | 1.00 | 0.003 | 1.00 | 1.00 |
| PRO50 | HB3 | 1.00 | 0.001 | 1.00 | 0.91 |
| PRO50 | HG2 | 1.00 | 0.002 | 1.00 | 6.41 |
| PRO50 | HG3 | 1.00 | 0.008 | 1.00 | 3.73 |
| PRO50 | HD2 | 1.00 | 0.000 | 1.00 | 0.42 |
| PRO50 | HD3 | 1.00 | 0.001 | 1.00 | 0.37 |

3.50.9 Detailed Probabilities of PRO50HG3:

Overall probability: 0.514

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO50 | 0.51 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P50HA | 1.00 |
| P50HB2 | 1.00 |
| P50HB3 | 1.00 |
| P50HG2 | 1.00 |
| P50HD2 | 1.00 |
| P50HD3 | 1.00 |
| P50HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO50 | HA | 1.00 | 0.034 | 0.60 | 0.00 |
| PRO50 | HB2 | 1.00 | 0.083 | 0.00 | 0.00 |
| PRO50 | HB3 | 1.00 | 0.049 | 0.00 | 0.00 |
| PRO50 | HG2 | 1.00 | 0.011 | 1.00 | 4.32 |
| PRO50 | HG3 | 1.00 | 0.018 | 1.00 | 31.34 |
| PRO50 | HD2 | 1.00 | 0.000 | 1.00 | 1.16 |
| PRO50 | HD3 | 1.00 | 0.046 | 0.00 | 0.00 |

3.50.10 Detailed Probabilities of PRO50HD2:

Overall probability: 0.822

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER49 | 0.76 | 1.00 |
| PRO50 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S49HA | 1.00 |
| S49H | 0.98 |
| S49HB3 | 0.97 |
| S49HB2 | 0.96 |
| P50HA | 1.00 |
| P50HB2 | 1.00 |
| P50HB3 | 1.00 |
| P50HG2 | 1.00 |
| P50HG3 | 1.00 |
| P50HD3 | 1.00 |
| P50HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER49 | HA | 1.00 | 0.009 | 1.00 | 0.53 |
| SER49 | HB2 | 0.96 | 0.149 | 0.04 | 0.00 |
| SER49 | HB3 | 0.97 | 0.009 | 1.00 | 0.14 |
| SER49 | H | 0.98 | 0.013 | 1.00 | -204631.00 |
| PRO50 | HA | 1.00 | 0.008 | 1.00 | 0.18 |
| PRO50 | HB2 | 1.00 | 0.013 | 1.00 | 0.88 |
| PRO50 | HB3 | 1.00 | 0.114 | 0.00 | 0.00 |
| PRO50 | HG2 | 1.00 | 0.000 | 1.00 | 0.80 |
| PRO50 | HG3 | 1.00 | 0.015 | 1.00 | 1.66 |
| PRO50 | HD2 | 1.00 | 0.013 | 1.00 | 8.06 |
| PRO50 | HD3 | 1.00 | 0.007 | 1.00 | 1.66 |

3.50.11 Detailed Probabilities of PRO50HD3:

Overall probability: 0.694

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER49 | 0.41 | 1.00 |
| PRO50 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S49HA | 1.00 |
| S49H | 0.96 |
| S49HB3 | 0.99 |
| S49HB2 | 0.98 |
| P50HA | 1.00 |
| P50HB2 | 1.00 |
| P50HB3 | 1.00 |
| P50HG2 | 1.00 |
| P50HG3 | 1.00 |
| P50HD2 | 1.00 |
| P50HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER49 | HA | 1.00 | 0.014 | 1.00 | 0.70 |
| SER49 | HB2 | 0.98 | 0.042 | 0.02 | 0.00 |
| SER49 | HB3 | 0.99 | 0.057 | 0.01 | 0.00 |
| SER49 | H | 0.96 | 0.034 | 0.60 | 0.00 |
| PRO50 | HA | 1.00 | 0.017 | 1.00 | 0.23 |
| PRO50 | HB2 | 1.00 | 0.004 | 1.00 | 0.22 |
| PRO50 | HB3 | 1.00 | 0.007 | 1.00 | 0.22 |
| PRO50 | HG2 | 1.00 | 0.006 | 1.00 | 0.70 |
| PRO50 | HG3 | 1.00 | 0.093 | 0.00 | 0.00 |
| PRO50 | HD2 | 1.00 | 0.004 | 1.00 | 1.62 |
| PRO50 | HD3 | 1.00 | 0.006 | 1.00 | 3.82 |

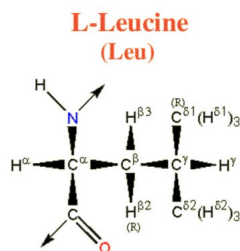
3.51 LEU(51)

Figure 41: Image from the BMRB

Residue probability: 0.934

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 177.161 | 177.056 | 1.929 | 0.000 | 0.000 |
| CA 3.51.1 | 56.713 | 55.735 | 3.802 | 0.845 | 1.000 |
| CB 3.51.2 | 38.569 | 42.389 | 3.750 | 1.000 | 1.000 |
| CG 3.51.3 | 26.770 | 26.892 | 3.086 | 0.875 | 1.000 |
| CD1 3.51.4 | 22.156 | 24.837 | 3.657 | 0.900 | 1.000 |
| CD2 3.51.5 | 25.243 | 24.201 | 3.117 | 1.000 | 1.000 |
| N 3.51.6 | 114.683 | 121.785 | 4.943 | 1.000 | 1.000 |
| HA 3.51.7 | 3.663 | 4.315 | 0.840 | 0.728 | 1.000 |
| HB2 3.51.8 | -0.386 | 1.601 | 0.373 | 1.000 | 1.000 |
| HB3 3.51.9 | 0.886 | 1.508 | 0.398 | 1.000 | 1.000 |
| HG 3.51.10 | 1.099 | 1.510 | 0.340 | 0.788 | 1.000 |
| HD1 3.51.11 | 0.559 | 0.739 | 0.294 | 1.000 | 1.000 |
| HD2 3.51.12 | 0.213 | 0.727 | 0.421 | 1.000 | 1.000 |
| H 3.51.13 | 6.438 | 8.237 | 0.647 | 1.000 | 1.000 |

3.51.1 Detailed Probabilities of LEU51CA:

Overall probability: 0.845

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO50 | 0.50 | 1.00 |
| LEU51 | 1.00 | 1.00 |
| ALA52 | 0.65 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P50HA | 1.00 |
| P50HB2 | 0.99 |
| L51HB2 | 1.00 |
| L51HB3 | 1.00 |
| L51HG | 1.00 |
| L51HD11 | 0.99 |
| L51HD21 | 0.99 |
| L51H | 1.00 |
| L51HA | 1.00 |
| A52HA | 1.00 |
| A52H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO50 | HA | 1.00 | 0.191 | 0.00 | 0.00 |
| PRO50 | HB2 | 0.99 | 0.023 | 1.00 | 0.51 |
| LEU51 | HA | 1.00 | 0.005 | 1.00 | 5.40 |
| LEU51 | HB2 | 1.00 | 0.006 | 1.00 | 0.65 |
| LEU51 | HB3 | 1.00 | 0.003 | 1.00 | 0.48 |
| LEU51 | HG | 1.00 | 0.019 | 1.00 | 0.28 |
| LEU51 | HD11 | 0.99 | 0.003 | 1.00 | 1.62 |
| LEU51 | HD21 | 0.99 | 0.002 | 1.00 | 0.28 |
| LEU51 | H | 1.00 | 0.001 | 1.00 | 0.43 |
| ALA52 | HA | 1.00 | 0.037 | 0.30 | 0.00 |
| ALA52 | H | 1.00 | 0.004 | 1.00 | 0.16 |

3.51.2 Detailed Probabilities of LEU51CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU51 | 1.00 | 1.00 |
| ALA52 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L51HA | 1.00 |
| L51HB3 | 1.00 |
| L51HG | 1.00 |
| L51HD11 | 1.00 |
| L51HD21 | 1.00 |
| L51H | 1.00 |
| L51HB2 | 1.00 |
| A52H | 1.00 |

NOESY contacts detailed probability

3.51 LEU(51)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU51 | HA | 1.00 | 0.006 | 1.00 | 0.31 |
| LEU51 | HB2 | 1.00 | 0.004 | 1.00 | 0.85 |
| LEU51 | HB3 | 1.00 | 0.002 | 1.00 | 0.78 |
| LEU51 | HG | 1.00 | 0.003 | 1.00 | 0.20 |
| LEU51 | HD11 | 1.00 | 0.010 | 1.00 | 0.43 |
| LEU51 | HD21 | 1.00 | 0.003 | 1.00 | 0.44 |
| LEU51 | H | 1.00 | 0.001 | 1.00 | 0.29 |
| ALA52 | H | 1.00 | 0.000 | 1.00 | 0.12 |

3.51.3 Detailed Probabilities of LEU51CG:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU51 | 0.86 | 1.00 |
| ALA52 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L51HA | 1.00 |
| L51HB2 | 1.00 |
| L51HB3 | 1.00 |
| L51HD11 | 1.00 |
| L51HD21 | 1.00 |
| L51H | 1.00 |
| L51HG | 1.00 |
| A52H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU51 | HA | 1.00 | 0.017 | 1.00 | 0.19 |
| LEU51 | HB2 | 1.00 | 0.001 | 1.00 | 0.20 |
| LEU51 | HB3 | 1.00 | 0.015 | 1.00 | 0.30 |
| LEU51 | HG | 1.00 | 0.228 | 0.00 | 0.00 |
| LEU51 | HD11 | 1.00 | 0.001 | 1.00 | 0.84 |
| LEU51 | HD21 | 1.00 | 0.003 | 1.00 | 0.70 |
| LEU51 | H | 1.00 | 0.002 | 1.00 | 0.08 |
| ALA52 | H | 0.98 | 0.003 | 1.00 | 0.10 |

3.51.4 Detailed Probabilities of LEU51CD1:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU51 | 0.90 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L51HA | 0.99 |
| L51HB2 | 1.00 |
| L51HB3 | 1.00 |
| L51HG | 1.00 |
| L51HD12 | 1.00 |
| L51HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU51 | HA | 0.99 | 0.006 | 1.00 | 2.69 |
| LEU51 | HB2 | 1.00 | 0.003 | 1.00 | 0.69 |
| LEU51 | HB3 | 1.00 | 0.003 | 1.00 | 1.15 |
| LEU51 | HG | 1.00 | 0.037 | 0.30 | 0.00 |
| LEU51 | HD11 | 1.00 | 0.001 | 1.00 | 63.83 |
| LEU51 | HD21 | 1.00 | 0.003 | 1.00 | 2.92 |
| LEU51 | H | 0.86 | 0.003 | 1.00 | 0.19 |

3.51.5 Detailed Probabilities of LEU51CD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU51 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L51HA | 0.99 |
| L51HB2 | 1.00 |
| L51HB3 | 1.00 |
| L51HG | 1.00 |
| L51HD11 | 1.00 |
| L51HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU51 | HA | 0.99 | 0.009 | 1.00 | 0.26 |
| LEU51 | HB2 | 1.00 | 0.003 | 1.00 | 0.67 |
| LEU51 | HB3 | 1.00 | 0.013 | 1.00 | 0.76 |
| LEU51 | HG | 1.00 | 0.001 | 1.00 | 1.06 |
| LEU51 | HD11 | 1.00 | 0.014 | 1.00 | 3.09 |
| LEU51 | HD21 | 1.00 | 0.003 | 1.00 | 27.22 |
| LEU51 | H | 0.85 | 0.003 | 1.00 | 0.19 |

3.51.6 Detailed Probabilities of LEU51N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO50 | 1.00 | 1.00 |
| LEU51 | 1.00 | 1.00 |
| ALA52 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P50HB2 | 1.00 |
| P50HA | 1.00 |
| P50HB3 | 1.00 |
| L51HA | 1.00 |
| L51HB2 | 1.00 |
| L51HB3 | 1.00 |
| L51HG | 1.00 |
| L51H | 1.00 |
| A52H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO50 | HA | 1.00 | 0.003 | 1.00 | -268312.00 |
| PRO50 | HB2 | 1.00 | 0.009 | 1.00 | -650405.00 |
| PRO50 | HB3 | 1.00 | 0.001 | 1.00 | -255925.00 |
| PRO50 | HG2 | 0.91 | 0.003 | 1.00 | -252320.00 |
| PRO50 | HD2 | 0.67 | 0.003 | 1.00 | -594575.00 |
| PRO50 | HD3 | 0.57 | 0.020 | 1.00 | -371084.00 |
| LEU51 | HA | 1.00 | 0.006 | 1.00 | -851403.00 |
| LEU51 | HB2 | 1.00 | 0.004 | 1.00 | -968377.00 |
| LEU51 | HB3 | 1.00 | 0.003 | 1.00 | -1282030.00 |
| LEU51 | HG | 1.00 | 0.007 | 1.00 | -239345.00 |
| LEU51 | H | 1.00 | 0.001 | 1.00 | -9205023.00 |
| LEU51 | HD11 | 0.88 | 0.024 | 1.00 | -637840.00 |
| LEU51 | HD21 | 0.87 | 0.004 | 1.00 | -405870.00 |
| ALA52 | H | 1.00 | 0.002 | 1.00 | -1340483.00 |

3.51.7 Detailed Probabilities of LEU51HA:

Overall probability: 0.728

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO50 | 0.51 | 1.00 |
| LEU51 | 1.00 | 1.00 |
| ALA52 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P50HA | 1.00 |
| P50HB2 | 0.99 |
| L51HB2 | 1.00 |
| L51HB3 | 1.00 |
| L51HG | 1.00 |
| L51HD11 | 0.99 |
| L51HD21 | 0.99 |
| L51H | 1.00 |
| L51HA | 1.00 |
| A52HA | 1.00 |
| A52H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO50 | HA | 1.00 | 0.008 | 1.00 | 0.09 |
| PRO50 | HB2 | 0.99 | 0.196 | 0.01 | 0.00 |
| LEU51 | HA | 1.00 | 0.005 | 1.00 | 5.40 |
| LEU51 | HB2 | 1.00 | 0.006 | 1.00 | 0.31 |
| LEU51 | HB3 | 1.00 | 0.005 | 1.00 | 0.24 |
| LEU51 | HG | 1.00 | 0.017 | 1.00 | 0.19 |
| LEU51 | HD11 | 0.99 | 0.006 | 1.00 | 2.69 |
| LEU51 | HD21 | 0.99 | 0.009 | 1.00 | 0.26 |
| LEU51 | H | 1.00 | 0.006 | 1.00 | -851403.00 |
| ALA52 | HA | 1.00 | 0.048 | 0.00 | 0.00 |
| ALA52 | H | 1.00 | 0.041 | 0.00 | 0.00 |

3.51.8 Detailed Probabilities of LEU51HB2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU51 | 1.00 | 1.00 |
| ALA52 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L51HA | 1.00 |
| L51HB3 | 1.00 |
| L51HG | 1.00 |
| L51HD11 | 1.00 |
| L51HD21 | 1.00 |
| L51H | 1.00 |
| L51HB2 | 1.00 |
| A52H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU51 | HA | 1.00 | 0.006 | 1.00 | 0.65 |
| LEU51 | HB2 | 1.00 | 0.004 | 1.00 | 0.85 |
| LEU51 | HB3 | 1.00 | 0.003 | 1.00 | 0.80 |
| LEU51 | HG | 1.00 | 0.001 | 1.00 | 0.20 |
| LEU51 | HD11 | 1.00 | 0.003 | 1.00 | 0.69 |
| LEU51 | HD21 | 1.00 | 0.003 | 1.00 | 0.67 |
| LEU51 | H | 1.00 | 0.004 | 1.00 | -968377.00 |
| ALA52 | H | 1.00 | 0.007 | 1.00 | -375077.00 |

3.51.9 Detailed Probabilities of LEU51HB3:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU51 | 1.00 | 1.00 |
| ALA52 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L51HA | 1.00 |
| L51HB2 | 1.00 |
| L51HG | 1.00 |
| L51HD11 | 1.00 |
| L51HD21 | 1.00 |
| L51H | 1.00 |
| L51HB3 | 1.00 |
| A52H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU51 | HA | 1.00 | 0.003 | 1.00 | 0.48 |
| LEU51 | HB2 | 1.00 | 0.002 | 1.00 | 0.78 |
| LEU51 | HB3 | 1.00 | 0.002 | 1.00 | 0.80 |
| LEU51 | HG | 1.00 | 0.015 | 1.00 | 0.30 |
| LEU51 | HD11 | 1.00 | 0.003 | 1.00 | 1.15 |
| LEU51 | HD21 | 1.00 | 0.013 | 1.00 | 0.76 |
| LEU51 | H | 1.00 | 0.003 | 1.00 | -1282030.00 |
| ALA52 | H | 1.00 | 0.001 | 1.00 | -650701.00 |

3.51.10 Detailed Probabilities of LEU51HG:

Overall probability: 0.788

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU51 | 0.76 | 1.00 |
| ALA52 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L51HA | 1.00 |
| L51HB2 | 1.00 |
| L51HB3 | 1.00 |
| L51HD11 | 1.00 |
| L51HD21 | 1.00 |
| L51H | 1.00 |
| L51HG | 1.00 |
| A52H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU51 | HA | 1.00 | 0.019 | 1.00 | 0.28 |
| LEU51 | HB2 | 1.00 | 0.003 | 1.00 | 0.20 |
| LEU51 | HB3 | 1.00 | 0.003 | 1.00 | 0.28 |
| LEU51 | HG | 1.00 | 0.228 | 0.00 | 0.00 |
| LEU51 | HD11 | 1.00 | 0.037 | 0.30 | 0.00 |
| LEU51 | HD21 | 1.00 | 0.001 | 1.00 | 1.06 |
| LEU51 | H | 1.00 | 0.007 | 1.00 | -239345.00 |
| ALA52 | H | 0.98 | 0.007 | 1.00 | -242686.00 |

3.51.11 Detailed Probabilities of LEU51HD11:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU51 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L51HA | 0.99 |
| L51HB2 | 1.00 |
| L51HB3 | 1.00 |
| L51HG | 1.00 |
| L51HD12 | 1.00 |
| L51HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU51 | HA | 0.99 | 0.003 | 1.00 | 1.62 |
| LEU51 | HB2 | 1.00 | 0.010 | 1.00 | 0.43 |
| LEU51 | HB3 | 1.00 | 0.011 | 1.00 | 0.38 |
| LEU51 | HG | 1.00 | 0.001 | 1.00 | 0.84 |
| LEU51 | HD11 | 1.00 | 0.001 | 1.00 | 63.83 |
| LEU51 | HD21 | 1.00 | 0.014 | 1.00 | 3.09 |
| LEU51 | H | 0.86 | 0.024 | 1.00 | -637840.00 |

3.51.12 Detailed Probabilities of LEU51HD21:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU51 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L51HA | 0.99 |
| L51HB2 | 1.00 |
| L51HB3 | 1.00 |
| L51HG | 1.00 |
| L51HD11 | 1.00 |
| L51HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU51 | HA | 0.99 | 0.002 | 1.00 | 0.28 |
| LEU51 | HB2 | 1.00 | 0.003 | 1.00 | 0.44 |
| LEU51 | HB3 | 1.00 | 0.003 | 1.00 | 0.47 |
| LEU51 | HG | 1.00 | 0.003 | 1.00 | 0.70 |
| LEU51 | HD11 | 1.00 | 0.003 | 1.00 | 2.92 |
| LEU51 | HD21 | 1.00 | 0.003 | 1.00 | 27.22 |
| LEU51 | H | 0.85 | 0.004 | 1.00 | -405870.00 |

3.51.13 Detailed Probabilities of LEU51H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO50 | 1.00 | 1.00 |
| LEU51 | 1.00 | 1.00 |
| ALA52 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P50HB2 | 1.00 |
| P50HA | 1.00 |
| P50HB3 | 1.00 |
| L51HA | 1.00 |
| L51HB2 | 1.00 |
| L51HB3 | 1.00 |
| L51HG | 1.00 |
| L51H | 1.00 |
| A52H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO50 | HA | 1.00 | 0.000 | 1.00 | 0.20 |
| PRO50 | HB2 | 1.00 | 0.001 | 1.00 | 0.20 |
| PRO50 | HB3 | 1.00 | 0.003 | 1.00 | 0.18 |
| PRO50 | HG2 | 0.91 | 0.002 | 1.00 | 0.21 |
| PRO50 | HG3 | 0.74 | 0.001 | 1.00 | 0.10 |
| PRO50 | HD2 | 0.67 | 0.002 | 1.00 | 0.15 |
| PRO50 | HD3 | 0.57 | 0.005 | 1.00 | 0.11 |
| LEU51 | HA | 1.00 | 0.001 | 1.00 | 0.43 |
| LEU51 | HB2 | 1.00 | 0.001 | 1.00 | 0.29 |
| LEU51 | HB3 | 1.00 | 0.000 | 1.00 | 0.37 |
| LEU51 | HG | 1.00 | 0.002 | 1.00 | 0.08 |
| LEU51 | H | 1.00 | 0.001 | 1.00 | -9205023.00 |
| LEU51 | HD11 | 0.88 | 0.003 | 1.00 | 0.19 |
| LEU51 | HD21 | 0.87 | 0.003 | 1.00 | 0.19 |
| ALA52 | H | 1.00 | 0.001 | 1.00 | -1268065.00 |

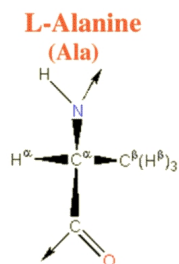
3.52 ALA(52)

Figure 42: Image from the BMRB

Residue probability: 0.941

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-----------|-------------|---------|--------|---------------------|--------------------|
| CA 3.52.1 | 55.692 | 53.289 | 3.425 | 0.846 | 1.000 |
| CB 3.52.2 | 16.298 | 19.355 | 4.103 | 1.000 | 1.000 |
| N 3.52.3 | 120.031 | 123.100 | 4.487 | 0.917 | 1.000 |
| HA 3.52.4 | 3.621 | 4.254 | 0.459 | 0.883 | 1.000 |
| HB 3.52.5 | 0.495 | 1.346 | 0.258 | 1.000 | 1.000 |
| H 3.52.6 | 7.245 | 8.206 | 0.601 | 1.000 | 1.000 |

3.52.1 Detailed Probabilities of ALA52CA:

Overall probability: 0.846

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU51 | 0.46 | 1.00 |
| ALA52 | 1.00 | 1.00 |
| ARG53 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L51HA | 1.00 |
| A52H | 1.00 |
| A52HB1 | 1.00 |
| A52HA | 1.00 |
| R53HA | 1.00 |
| R53H | 1.00 |

NOESY contacts detailed probability

3.52 ALA(52)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU51 | HA | 1.00 | 0.048 | 0.00 | 0.00 |
| LEU51 | HB3 | 0.92 | 0.032 | 0.92 | 0.00 |
| ALA52 | HA | 1.00 | 0.006 | 1.00 | 6.25 |
| ALA52 | HB1 | 1.00 | 0.001 | 1.00 | 1.59 |
| ALA52 | H | 1.00 | 0.005 | 1.00 | 0.49 |
| ARG53 | HA | 1.00 | 0.011 | 1.00 | 0.07 |
| ARG53 | H | 1.00 | 0.001 | 1.00 | 0.15 |

3.52.2 Detailed Probabilities of ALA52CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA52 | 1.00 | 1.00 |
| ARG53 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A52HA | 1.00 |
| A52H | 1.00 |
| A52HB2 | 1.00 |
| R53H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA52 | HA | 1.00 | 0.005 | 1.00 | 1.14 |
| ALA52 | HB1 | 1.00 | 0.004 | 1.00 | 15.78 |
| ALA52 | H | 1.00 | 0.007 | 1.00 | 0.88 |
| ARG53 | H | 1.00 | 0.003 | 1.00 | 0.40 |
| ARG53 | HA | 0.69 | 0.019 | 1.00 | 0.44 |

3.52.3 Detailed Probabilities of ALA52N:

Overall probability: 0.917

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU51 | 0.83 | 1.00 |
| ALA52 | 1.00 | 1.00 |
| ARG53 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L51HG | 0.98 |
| L51HB3 | 1.00 |
| L51H | 1.00 |
| L51HA | 1.00 |
| L51HB2 | 1.00 |
| A52HA | 1.00 |
| A52HB1 | 1.00 |
| A52H | 1.00 |
| R53H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU51 | HA | 1.00 | 0.041 | 0.00 | 0.00 |
| LEU51 | HB2 | 1.00 | 0.007 | 1.00 | -375077.00 |
| LEU51 | HB3 | 1.00 | 0.001 | 1.00 | -650701.00 |
| LEU51 | HG | 0.98 | 0.007 | 1.00 | -242686.00 |
| LEU51 | H | 1.00 | 0.001 | 1.00 | -1268065.00 |
| LEU51 | HD21 | 0.58 | 0.002 | 1.00 | -245374.00 |
| ALA52 | HA | 1.00 | 0.001 | 1.00 | -938763.00 |
| ALA52 | HB1 | 1.00 | 0.000 | 1.00 | -2132308.00 |
| ALA52 | H | 1.00 | 0.005 | 1.00 | -10122184.00 |
| ARG53 | H | 1.00 | 0.002 | 1.00 | -991886.00 |
| ARG53 | HA | 0.87 | 0.019 | 1.00 | -455793.00 |
| ARG53 | HB2 | 0.56 | 0.003 | 1.00 | -81358.00 |

3.52.4 Detailed Probabilities of ALA52HA:

Overall probability: 0.883

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU51 | 0.30 | 1.00 |
| ALA52 | 1.00 | 1.00 |
| ARG53 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L51HA | 1.00 |
| A52H | 1.00 |
| A52HB1 | 1.00 |
| A52HA | 1.00 |
| R53HA | 1.00 |
| R53H | 1.00 |

NOESY contacts detailed probability

3.52 ALA(52)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU51 | HA | 1.00 | 0.037 | 0.30 | 0.00 |
| ALA52 | HA | 1.00 | 0.006 | 1.00 | 6.25 |
| ALA52 | HB1 | 1.00 | 0.005 | 1.00 | 1.14 |
| ALA52 | H | 1.00 | 0.001 | 1.00 | -938763.00 |
| ARG53 | HA | 1.00 | 0.014 | 1.00 | 0.07 |
| ARG53 | H | 1.00 | 0.000 | 1.00 | -410651.00 |

3.52.5 Detailed Probabilities of ALA52HB1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA52 | 1.00 | 1.00 |
| ARG53 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A52HA | 1.00 |
| A52H | 1.00 |
| A52HB2 | 1.00 |
| R53H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA52 | HA | 1.00 | 0.001 | 1.00 | 1.59 |
| ALA52 | HB1 | 1.00 | 0.004 | 1.00 | 15.78 |
| ALA52 | H | 1.00 | 0.000 | 1.00 | -2132308.00 |
| ARG53 | H | 1.00 | 0.002 | 1.00 | -1445919.00 |
| ARG53 | HA | 0.69 | 0.004 | 1.00 | 0.13 |

3.52.6 Detailed Probabilities of ALA52H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU51 | 1.00 | 1.00 |
| ALA52 | 1.00 | 1.00 |
| ARG53 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L51HG | 0.98 |
| L51HB3 | 1.00 |
| L51H | 1.00 |
| L51HA | 1.00 |
| L51HB2 | 1.00 |
| A52HA | 1.00 |
| A52HB1 | 1.00 |
| A52H | 1.00 |
| R53H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU51 | HA | 1.00 | 0.004 | 1.00 | 0.16 |
| LEU51 | HB2 | 1.00 | 0.000 | 1.00 | 0.12 |
| LEU51 | HB3 | 1.00 | 0.005 | 1.00 | 0.17 |
| LEU51 | HG | 0.98 | 0.003 | 1.00 | 0.10 |
| LEU51 | H | 1.00 | 0.002 | 1.00 | -1340483.00 |
| LEU51 | HD21 | 0.58 | 0.016 | 1.00 | 0.32 |
| ALA52 | HA | 1.00 | 0.005 | 1.00 | 0.49 |
| ALA52 | HB1 | 1.00 | 0.007 | 1.00 | 0.88 |
| ALA52 | H | 1.00 | 0.005 | 1.00 | -10122184.00 |
| ARG53 | H | 1.00 | 0.005 | 1.00 | -1406074.00 |

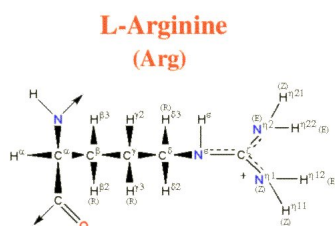


Figure 43: Image from the BMRB

Residue probability: 0.872
 Residue probability confidence: 0.866

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 178.539 | 176.453 | 2.303 | 0.000 | 0.000 |
| CA 3.53.1 | 59.924 | 56.803 | 3.326 | 1.000 | 1.000 |
| CB 3.53.2 | 29.843 | 30.892 | 2.424 | 1.000 | 0.900 |
| CG 3.53.3 | 27.310 | 27.247 | 1.538 | 1.000 | 0.818 |
| CD 3.53.4 | 43.754 | 43.189 | 1.415 | 0.750 | 0.700 |
| N 3.53.5 | 115.531 | 120.701 | 3.779 | 1.000 | 1.000 |
| NE | NA | – | – | 0.000 | 0.000 |
| NH1 | NA | – | – | 0.000 | 0.000 |
| NH2 | NA | – | – | 0.000 | 0.000 |
| HA 3.53.6 | 3.800 | 4.301 | 0.495 | 0.923 | 1.000 |
| HB2 3.53.7 | 1.938 | 1.793 | 0.292 | 0.778 | 0.900 |
| HB3 3.53.8 | 1.809 | 1.757 | 0.307 | 1.000 | 0.900 |
| HG2 3.53.9 | 1.464 | 1.559 | 0.294 | 0.889 | 0.818 |
| HG3 3.53.10 | 1.792 | 1.535 | 0.310 | 1.000 | 0.818 |
| HD2 3.53.11 | 3.101 | 3.105 | 0.301 | 0.500 | 0.700 |
| HD3 3.53.12 | 3.104 | 3.081 | 0.306 | 0.500 | 0.700 |
| H 3.53.13 | 8.367 | 8.248 | 0.623 | 1.000 | 1.000 |
| HE | NA | – | – | 0.000 | 0.000 |
| HH1 | NA | – | – | 0.000 | 0.000 |
| HH2 | NA | – | – | 0.000 | 0.000 |

3.53.1 Detailed Probabilities of ARG53CA:

Overall probability: 1.000
 Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA52 | 1.00 | 1.00 |
| ARG53 | 1.00 | 1.00 |
| GLN54 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A52HA | 1.00 |
| R53HB2 | 1.00 |
| R53HB3 | 1.00 |
| R53HG2 | 1.00 |
| R53HG3 | 1.00 |
| R53HD2 | 0.98 |
| R53HD3 | 0.97 |
| R53H | 1.00 |
| R53HA | 1.00 |
| Q54HA | 1.00 |
| Q54H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA52 | HA | 1.00 | 0.014 | 1.00 | 0.07 |
| ALA52 | HB1 | 0.67 | 0.004 | 1.00 | 0.13 |
| ARG53 | HA | 1.00 | 0.001 | 1.00 | 8.11 |
| ARG53 | HB2 | 1.00 | 0.004 | 1.00 | 0.98 |
| ARG53 | HB3 | 1.00 | 0.009 | 1.00 | 1.21 |
| ARG53 | HG2 | 1.00 | 0.004 | 1.00 | 0.52 |
| ARG53 | HG3 | 1.00 | 0.008 | 1.00 | 1.21 |
| ARG53 | HD2 | 0.98 | 0.000 | 1.00 | 0.27 |
| ARG53 | HD3 | 0.97 | 0.003 | 1.00 | 0.27 |
| ARG53 | H | 1.00 | 0.000 | 1.00 | 0.63 |
| GLN54 | HA | 1.00 | 0.005 | 1.00 | 0.16 |
| GLN54 | H | 1.00 | 0.003 | 1.00 | 0.22 |

3.53.2 Detailed Probabilities of ARG53CB:

Overall probability: 1.000

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG53 | 1.00 | 0.89 |
| GLN54 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R53HA | 1.00 |
| R53HB2 | 1.00 |
| R53HG2 | 1.00 |
| R53HG3 | 1.00 |
| R53HD2 | 1.00 |
| R53HD3 | 1.00 |
| R53H | 1.00 |
| R53HE | 1.00 |
| R53HB3 | 1.00 |
| Q54H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG53 | HA | 1.00 | 0.003 | 1.00 | 0.61 |
| ARG53 | HB2 | 1.00 | 0.002 | 1.00 | 2.94 |
| ARG53 | HB3 | 1.00 | 0.007 | 1.00 | 5.78 |
| ARG53 | HG2 | 1.00 | 0.001 | 1.00 | 1.09 |
| ARG53 | HG3 | 1.00 | 0.010 | 1.00 | 5.78 |
| ARG53 | HD2 | 1.00 | 0.001 | 1.00 | 0.69 |
| ARG53 | HD3 | 1.00 | 0.004 | 1.00 | 0.69 |
| ARG53 | H | 1.00 | 0.001 | 1.00 | 0.61 |
| GLN54 | H | 1.00 | 0.001 | 1.00 | 0.39 |
| GLN54 | HA | 0.79 | 0.000 | 1.00 | 0.12 |

3.53.3 Detailed Probabilities of ARG53CG:

Overall probability: 1.000

Overall confidence: 0.818

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG53 | 1.00 | 0.80 |
| GLN54 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R53HA | 1.00 |
| R53HB2 | 1.00 |
| R53HB3 | 1.00 |
| R53HG2 | 1.00 |
| R53HD2 | 1.00 |
| R53HD3 | 1.00 |
| R53H | 1.00 |
| R53HE | 1.00 |
| R53HH11 | 1.00 |
| R53HG3 | 1.00 |
| Q54H | 0.96 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG53 | HA | 1.00 | 0.007 | 1.00 | 0.57 |
| ARG53 | HB2 | 1.00 | 0.005 | 1.00 | 1.67 |
| ARG53 | HB3 | 1.00 | 0.016 | 1.00 | 9.47 |
| ARG53 | HG2 | 1.00 | 0.002 | 1.00 | 4.01 |
| ARG53 | HG3 | 1.00 | 0.001 | 1.00 | 9.47 |
| ARG53 | HD2 | 1.00 | 0.000 | 1.00 | 1.12 |
| ARG53 | HD3 | 1.00 | 0.003 | 1.00 | 1.12 |
| ARG53 | H | 1.00 | 0.002 | 1.00 | 0.50 |
| GLN54 | H | 0.96 | 0.000 | 1.00 | 0.19 |

3.53.4 Detailed Probabilities of ARG53CD:

Overall probability: 0.750

Overall confidence: 0.700

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG53 | 0.75 | 0.70 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R53HA | 0.98 |
| R53HB2 | 1.00 |
| R53HB3 | 1.00 |
| R53HG2 | 1.00 |
| R53HG3 | 1.00 |
| R53HD3 | 1.00 |
| R53HE | 1.00 |
| R53HH11 | 1.00 |
| R53HH21 | 1.00 |
| R53HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG53 | HA | 0.98 | 0.002 | 1.00 | 0.22 |
| ARG53 | HB2 | 1.00 | 0.002 | 1.00 | 1.07 |
| ARG53 | HB3 | 1.00 | 0.014 | 1.00 | 1.80 |
| ARG53 | HG2 | 1.00 | 0.003 | 1.00 | 1.59 |
| ARG53 | HG3 | 1.00 | 0.003 | 1.00 | 1.80 |
| ARG53 | HD2 | 1.00 | 0.121 | 0.00 | 0.00 |
| ARG53 | HD3 | 1.00 | 0.124 | 0.00 | 0.00 |
| ARG53 | H | 0.87 | 0.004 | 1.00 | 0.14 |

3.53.5 Detailed Probabilities of ARG53N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA52 | 1.00 | 1.00 |
| ARG53 | 1.00 | 1.00 |
| GLN54 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A52HA | 1.00 |
| A52HB2 | 1.00 |
| A52H | 1.00 |
| R53HA | 1.00 |
| R53HB2 | 1.00 |
| R53HB3 | 1.00 |
| R53HG2 | 1.00 |
| R53HG3 | 1.00 |
| R53H | 1.00 |
| Q54H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA52 | HA | 1.00 | 0.000 | 1.00 | -410651.00 |
| ALA52 | HB1 | 1.00 | 0.002 | 1.00 | -1445919.00 |
| ALA52 | H | 1.00 | 0.005 | 1.00 | -1406074.00 |
| ARG53 | HA | 1.00 | 0.004 | 1.00 | -1263452.00 |
| ARG53 | HB2 | 1.00 | 0.005 | 1.00 | -1877262.00 |
| ARG53 | HB3 | 1.00 | 0.007 | 1.00 | -2189370.00 |
| ARG53 | HG2 | 1.00 | 0.000 | 1.00 | -450636.00 |
| ARG53 | HG3 | 1.00 | 0.010 | 1.00 | -2189370.00 |
| ARG53 | H | 1.00 | 0.001 | 1.00 | -13474470.00 |
| ARG53 | HD2 | 0.87 | 0.002 | 1.00 | -250427.00 |
| ARG53 | HD3 | 0.86 | 0.001 | 1.00 | -250427.00 |
| GLN54 | H | 1.00 | 0.000 | 1.00 | -1145175.00 |
| GLN54 | HA | 0.90 | 0.010 | 1.00 | -125114.00 |
| GLN54 | HB2 | 0.61 | 0.007 | 1.00 | -217886.00 |

3.53.6 Detailed Probabilities of ARG53HA:

Overall probability: 0.923

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA52 | 1.00 | 1.00 |
| ARG53 | 1.00 | 1.00 |
| GLN54 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A52HA | 1.00 |
| R53HB2 | 1.00 |
| R53HB3 | 1.00 |
| R53HG2 | 1.00 |
| R53HG3 | 1.00 |
| R53HD2 | 0.98 |
| R53HD3 | 0.97 |
| R53H | 1.00 |
| R53HA | 1.00 |
| Q54HA | 1.00 |
| Q54H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA52 | HA | 1.00 | 0.011 | 1.00 | 0.07 |
| ALA52 | HB1 | 0.67 | 0.019 | 1.00 | 0.44 |
| ALA52 | H | 0.87 | 0.019 | 1.00 | -455793.00 |
| ARG53 | HA | 1.00 | 0.001 | 1.00 | 8.11 |
| ARG53 | HB2 | 1.00 | 0.003 | 1.00 | 0.71 |
| ARG53 | HB3 | 1.00 | 0.003 | 1.00 | 0.61 |
| ARG53 | HG2 | 1.00 | 0.003 | 1.00 | 1.03 |
| ARG53 | HG3 | 1.00 | 0.007 | 1.00 | 0.57 |
| ARG53 | HD2 | 0.98 | 0.002 | 1.00 | 0.22 |
| ARG53 | HD3 | 0.97 | 0.002 | 1.00 | 0.22 |
| ARG53 | H | 1.00 | 0.004 | 1.00 | -1263452.00 |
| GLN54 | HA | 1.00 | 0.136 | 0.00 | 0.00 |
| GLN54 | H | 1.00 | 0.001 | 1.00 | -425060.00 |

3.53.7 Detailed Probabilities of ARG53HB2:

Overall probability: 0.778

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG53 | 0.75 | 0.89 |
| GLN54 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R53HA | 1.00 |
| R53HB3 | 1.00 |
| R53HG2 | 1.00 |
| R53HG3 | 1.00 |
| R53HD2 | 1.00 |
| R53HD3 | 1.00 |
| R53H | 1.00 |
| R53HE | 1.00 |
| R53HB2 | 1.00 |
| Q54H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG53 | HA | 1.00 | 0.004 | 1.00 | 0.98 |
| ARG53 | HB2 | 1.00 | 0.135 | 0.00 | 0.00 |
| ARG53 | HB3 | 1.00 | 0.002 | 1.00 | 2.94 |
| ARG53 | HG2 | 1.00 | 0.145 | 0.00 | 0.00 |
| ARG53 | HG3 | 1.00 | 0.005 | 1.00 | 1.67 |
| ARG53 | HD2 | 1.00 | 0.002 | 1.00 | 1.07 |
| ARG53 | HD3 | 1.00 | 0.002 | 1.00 | 1.07 |
| ARG53 | H | 1.00 | 0.005 | 1.00 | -1877262.00 |
| GLN54 | H | 1.00 | 0.006 | 1.00 | -888687.00 |

3.53.8 Detailed Probabilities of ARG53HB3:

Overall probability: 1.000

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG53 | 1.00 | 0.89 |
| GLN54 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R53HA | 1.00 |
| R53HB2 | 1.00 |
| R53HG2 | 1.00 |
| R53HG3 | 1.00 |
| R53HD2 | 1.00 |
| R53HD3 | 1.00 |
| R53H | 1.00 |
| R53HE | 1.00 |
| R53HB3 | 1.00 |
| Q54H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG53 | HA | 1.00 | 0.009 | 1.00 | 1.21 |
| ARG53 | HB2 | 1.00 | 0.006 | 1.00 | 4.59 |
| ARG53 | HB3 | 1.00 | 0.007 | 1.00 | 5.78 |
| ARG53 | HG2 | 1.00 | 0.016 | 1.00 | 5.37 |
| ARG53 | HG3 | 1.00 | 0.016 | 1.00 | 9.47 |
| ARG53 | HD2 | 1.00 | 0.014 | 1.00 | 1.80 |
| ARG53 | HD3 | 1.00 | 0.014 | 1.00 | 1.80 |
| ARG53 | H | 1.00 | 0.007 | 1.00 | -2189370.00 |
| GLN54 | H | 1.00 | 0.004 | 1.00 | -1096904.00 |

3.53.9 Detailed Probabilities of ARG53HG2:

Overall probability: 0.889

Overall confidence: 0.818

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG53 | 0.88 | 0.80 |
| GLN54 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R53HA | 1.00 |
| R53HB2 | 1.00 |
| R53HB3 | 1.00 |
| R53HG3 | 1.00 |
| R53HD2 | 1.00 |
| R53HD3 | 1.00 |
| R53H | 1.00 |
| R53HE | 1.00 |
| R53HH11 | 1.00 |
| R53HG2 | 1.00 |
| Q54H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG53 | HA | 1.00 | 0.004 | 1.00 | 0.52 |
| ARG53 | HB2 | 1.00 | 0.001 | 1.00 | 0.70 |
| ARG53 | HB3 | 1.00 | 0.001 | 1.00 | 1.09 |
| ARG53 | HG2 | 1.00 | 0.173 | 0.00 | 0.00 |
| ARG53 | HG3 | 1.00 | 0.002 | 1.00 | 4.01 |
| ARG53 | HD2 | 1.00 | 0.003 | 1.00 | 1.59 |
| ARG53 | HD3 | 1.00 | 0.003 | 1.00 | 1.59 |
| ARG53 | H | 1.00 | 0.000 | 1.00 | -450636.00 |
| GLN54 | H | 0.97 | 0.004 | 1.00 | -163878.00 |

3.53.10 Detailed Probabilities of ARG53HG3:

Overall probability: 1.000

Overall confidence: 0.818

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG53 | 1.00 | 0.80 |
| GLN54 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R53HA | 1.00 |
| R53HB2 | 1.00 |
| R53HB3 | 1.00 |
| R53HG2 | 1.00 |
| R53HD2 | 1.00 |
| R53HD3 | 1.00 |
| R53H | 1.00 |
| R53HE | 1.00 |
| R53HH11 | 1.00 |
| R53HG3 | 1.00 |
| Q54H | 0.96 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG53 | HA | 1.00 | 0.008 | 1.00 | 1.21 |
| ARG53 | HB2 | 1.00 | 0.011 | 1.00 | 4.59 |
| ARG53 | HB3 | 1.00 | 0.010 | 1.00 | 5.78 |
| ARG53 | HG2 | 1.00 | 0.001 | 1.00 | 5.37 |
| ARG53 | HG3 | 1.00 | 0.001 | 1.00 | 9.47 |
| ARG53 | HD2 | 1.00 | 0.003 | 1.00 | 1.80 |
| ARG53 | HD3 | 1.00 | 0.003 | 1.00 | 1.80 |
| ARG53 | H | 1.00 | 0.010 | 1.00 | -2189370.00 |
| GLN54 | H | 0.96 | 0.013 | 1.00 | -1096904.00 |

3.53.11 Detailed Probabilities of ARG53HD2:

Overall probability: 0.500

Overall confidence: 0.700

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG53 | 0.50 | 0.70 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R53HA | 0.98 |
| R53HB2 | 1.00 |
| R53HB3 | 1.00 |
| R53HG2 | 1.00 |
| R53HG3 | 1.00 |
| R53HD3 | 1.00 |
| R53HE | 1.00 |
| R53HH11 | 1.00 |
| R53HH21 | 1.00 |
| R53HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG53 | HA | 0.98 | 0.000 | 1.00 | 0.27 |
| ARG53 | HB2 | 1.00 | 0.421 | 0.00 | 0.00 |
| ARG53 | HB3 | 1.00 | 0.001 | 1.00 | 0.69 |
| ARG53 | HG2 | 1.00 | 0.113 | 0.00 | 0.00 |
| ARG53 | HG3 | 1.00 | 0.000 | 1.00 | 1.12 |
| ARG53 | HD2 | 1.00 | 0.121 | 0.00 | 0.00 |
| ARG53 | HD3 | 1.00 | 0.121 | 0.00 | 0.00 |
| ARG53 | H | 0.87 | 0.002 | 1.00 | -250427.00 |

3.53.12 Detailed Probabilities of ARG53HD3:

Overall probability: 0.500

Overall confidence: 0.700

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG53 | 0.50 | 0.70 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R53HA | 0.97 |
| R53HB2 | 1.00 |
| R53HB3 | 1.00 |
| R53HG2 | 1.00 |
| R53HG3 | 1.00 |
| R53HD2 | 1.00 |
| R53HE | 1.00 |
| R53HH11 | 1.00 |
| R53HH21 | 1.00 |
| R53HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG53 | HA | 0.97 | 0.003 | 1.00 | 0.27 |
| ARG53 | HB2 | 1.00 | 0.418 | 0.00 | 0.00 |
| ARG53 | HB3 | 1.00 | 0.004 | 1.00 | 0.69 |
| ARG53 | HG2 | 1.00 | 0.110 | 0.00 | 0.00 |
| ARG53 | HG3 | 1.00 | 0.003 | 1.00 | 1.12 |
| ARG53 | HD2 | 1.00 | 0.124 | 0.00 | 0.00 |
| ARG53 | HD3 | 1.00 | 0.124 | 0.00 | 0.00 |
| ARG53 | H | 0.86 | 0.001 | 1.00 | -250427.00 |

3.53.13 Detailed Probabilities of ARG53H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA52 | 1.00 | 1.00 |
| ARG53 | 1.00 | 1.00 |
| GLN54 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A52HA | 1.00 |
| A52HB2 | 1.00 |
| A52H | 1.00 |
| R53HA | 1.00 |
| R53HB2 | 1.00 |
| R53HB3 | 1.00 |
| R53HG2 | 1.00 |
| R53HG3 | 1.00 |
| R53H | 1.00 |
| Q54H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA52 | HA | 1.00 | 0.001 | 1.00 | 0.15 |
| ALA52 | HB1 | 1.00 | 0.003 | 1.00 | 0.40 |
| ALA52 | H | 1.00 | 0.002 | 1.00 | -991886.00 |
| ARG53 | HA | 1.00 | 0.000 | 1.00 | 0.63 |
| ARG53 | HB2 | 1.00 | 0.002 | 1.00 | 0.74 |
| ARG53 | HB3 | 1.00 | 0.001 | 1.00 | 0.61 |
| ARG53 | HG2 | 1.00 | 0.002 | 1.00 | 0.33 |
| ARG53 | HG3 | 1.00 | 0.002 | 1.00 | 0.50 |
| ARG53 | H | 1.00 | 0.001 | 1.00 | -13474470.00 |
| ARG53 | HD2 | 0.87 | 0.004 | 1.00 | 0.14 |
| ARG53 | HD3 | 0.86 | 0.004 | 1.00 | 0.14 |
| GLN54 | H | 1.00 | 0.001 | 1.00 | -1071373.00 |
| GLN54 | HB2 | 0.61 | 0.000 | 1.00 | 0.09 |

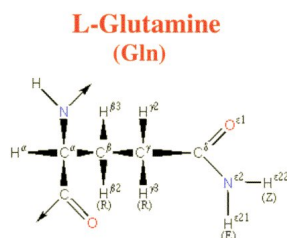
3.54 GLN(54)

Figure 44: Image from the BMRB

Residue probability: 0.818

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|--------------|-------------|---------|--------|---------------------|--------------------|
| C | 179.709 | 176.405 | 1.998 | 0.000 | 0.000 |
| CA 3.54.1 | 58.530 | 56.667 | 2.318 | 0.667 | 1.000 |
| CB 3.54.2 | 28.314 | 29.436 | 2.799 | 0.600 | 1.000 |
| CG 3.54.3 | 33.720 | 33.781 | 1.871 | 0.889 | 1.000 |
| N 3.54.4 | 116.358 | 119.799 | 3.762 | 1.000 | 1.000 |
| NE2 3.54.5 | 110.197 | 111.924 | 2.434 | 1.000 | 1.000 |
| HA 3.54.6 | 4.001 | 4.265 | 0.455 | 0.917 | 1.000 |
| HB2 3.54.7 | 2.076 | 2.047 | 0.290 | 0.778 | 1.000 |
| HB3 3.54.8 | 2.077 | 2.012 | 0.313 | 0.778 | 1.000 |
| HG2 3.54.9 | 2.539 | 2.308 | 0.289 | 1.000 | 1.000 |
| HG3 3.54.10 | 2.638 | 2.284 | 0.313 | 1.000 | 1.000 |
| H 3.54.11 | 7.495 | 8.232 | 0.711 | 1.000 | 1.000 |
| HE21 3.54.12 | 7.422 | 7.217 | 0.496 | 0.333 | 1.000 |
| HE22 3.54.13 | 6.871 | 7.041 | 0.463 | 0.667 | 1.000 |

3.54.1 Detailed Probabilities of GLN54CA:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG53 | 0.00 | 1.00 |
| GLN54 | 0.83 | 1.00 |
| LEU55 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R53HA | 1.00 |
| Q54HB2 | 1.00 |
| Q54HB3 | 1.00 |
| Q54HG2 | 1.00 |
| Q54HG3 | 1.00 |
| Q54H | 1.00 |
| Q54HA | 1.00 |
| L55H | 1.00 |
| L55HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG53 | HA | 1.00 | 0.136 | 0.00 | 0.00 |
| GLN54 | HA | 1.00 | 0.337 | 0.00 | 0.00 |
| GLN54 | HB2 | 1.00 | 0.012 | 1.00 | 2.76 |
| GLN54 | HB3 | 1.00 | 0.013 | 1.00 | 2.76 |
| GLN54 | HG2 | 1.00 | 0.006 | 1.00 | 0.69 |
| GLN54 | HG3 | 1.00 | 0.004 | 1.00 | 0.44 |
| GLN54 | H | 1.00 | 0.003 | 1.00 | 0.73 |
| LEU55 | HA | 1.00 | 0.362 | 0.00 | 0.00 |
| LEU55 | H | 1.00 | 0.002 | 1.00 | 0.30 |

3.54.2 Detailed Probabilities of GLN54CB:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN54 | 0.50 | 1.00 |
| LEU55 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q54HA | 1.00 |
| Q54HB3 | 1.00 |
| Q54HG2 | 1.00 |
| Q54HG3 | 1.00 |
| Q54H | 1.00 |
| Q54HE21 | 1.00 |
| Q54HE22 | 1.00 |
| Q54HB2 | 1.00 |
| L55H | 1.00 |

NOESY contacts detailed probability

3.54 GLN(54)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN54 | HA | 1.00 | 0.002 | 1.00 | 1.17 |
| GLN54 | HB2 | 1.00 | 0.472 | 0.00 | 0.00 |
| GLN54 | HB3 | 1.00 | 0.471 | 0.00 | 0.00 |
| GLN54 | HG2 | 1.00 | 0.009 | 1.00 | 0.91 |
| GLN54 | HG3 | 1.00 | 0.000 | 1.00 | 0.94 |
| GLN54 | H | 1.00 | 0.003 | 1.00 | 0.90 |
| GLN54 | HE21 | 1.00 | 0.076 | 0.00 | 0.00 |
| GLN54 | HE22 | 1.00 | 0.055 | 0.00 | 0.00 |
| LEU55 | H | 1.00 | 0.006 | 1.00 | 0.41 |
| LEU55 | HA | 0.87 | 0.027 | 1.00 | 1.17 |

3.54.3 Detailed Probabilities of GLN54CG:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN54 | 0.88 | 1.00 |
| LEU55 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q54HA | 1.00 |
| Q54HB2 | 1.00 |
| Q54HB3 | 1.00 |
| Q54HG3 | 1.00 |
| Q54H | 1.00 |
| Q54HE21 | 1.00 |
| Q54HE22 | 1.00 |
| Q54HG2 | 1.00 |
| L55H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN54 | HA | 1.00 | 0.002 | 1.00 | 0.82 |
| GLN54 | HB2 | 1.00 | 0.004 | 1.00 | 1.90 |
| GLN54 | HB3 | 1.00 | 0.005 | 1.00 | 1.90 |
| GLN54 | HG2 | 1.00 | 0.005 | 1.00 | 12.43 |
| GLN54 | HG3 | 1.00 | 0.000 | 1.00 | 9.00 |
| GLN54 | H | 1.00 | 0.002 | 1.00 | 0.73 |
| GLN54 | HE21 | 1.00 | 0.071 | 0.00 | 0.00 |
| GLN54 | HE22 | 1.00 | 0.000 | 1.00 | 0.11 |
| LEU55 | H | 0.98 | 0.000 | 1.00 | 0.13 |

3.54.4 Detailed Probabilities of GLN54N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG53 | 1.00 | 1.00 |
| GLN54 | 1.00 | 1.00 |
| LEU55 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R53H | 1.00 |
| R53HB2 | 1.00 |
| R53HG2 | 0.97 |
| R53HG3 | 0.96 |
| R53HA | 1.00 |
| R53HB3 | 1.00 |
| Q54HA | 1.00 |
| Q54HB2 | 1.00 |
| Q54HB3 | 1.00 |
| Q54HG2 | 1.00 |
| Q54HG3 | 1.00 |
| Q54H | 1.00 |
| L55H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG53 | HA | 1.00 | 0.001 | 1.00 | -425060.00 |
| ARG53 | HB2 | 1.00 | 0.006 | 1.00 | -888687.00 |
| ARG53 | HB3 | 1.00 | 0.004 | 1.00 | -1096904.00 |
| ARG53 | HG2 | 0.97 | 0.004 | 1.00 | -163878.00 |
| ARG53 | HG3 | 0.96 | 0.013 | 1.00 | -1096904.00 |
| ARG53 | H | 1.00 | 0.001 | 1.00 | -1071373.00 |
| GLN54 | HA | 1.00 | 0.002 | 1.00 | -1374715.00 |
| GLN54 | HB2 | 1.00 | 0.003 | 1.00 | -3003286.00 |
| GLN54 | HB3 | 1.00 | 0.004 | 1.00 | -3003286.00 |
| GLN54 | HG2 | 1.00 | 0.007 | 1.00 | -1247489.00 |
| GLN54 | HG3 | 1.00 | 0.000 | 1.00 | -1226057.00 |
| GLN54 | H | 1.00 | 0.002 | 1.00 | -14186829.00 |
| LEU55 | H | 1.00 | 0.005 | 1.00 | -1668657.00 |
| LEU55 | HA | 0.94 | 0.027 | 1.00 | -1374715.00 |

3.54.5 Detailed Probabilities of GLN54NE2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN54 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q54HB2 | 1.00 |
| Q54HB3 | 1.00 |
| Q54HG2 | 1.00 |
| Q54HG3 | 1.00 |
| Q54HE22 | 1.00 |
| Q54HE21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN54 | HB2 | 1.00 | 0.012 | 1.00 | -332928.00 |
| GLN54 | HB3 | 1.00 | 0.013 | 1.00 | -332928.00 |
| GLN54 | HG2 | 1.00 | 0.005 | 1.00 | -515743.00 |
| GLN54 | HG3 | 1.00 | 0.002 | 1.00 | -743910.00 |
| GLN54 | HE21 | 1.00 | 0.004 | 1.00 | -22583980.00 |
| GLN54 | HE22 | 1.00 | 0.001 | 1.00 | -14435378.00 |
| GLN54 | HA | 0.94 | 0.016 | 1.00 | -147438.00 |

3.54.6 Detailed Probabilities of GLN54HA:

Overall probability: 0.917

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG53 | 1.00 | 1.00 |
| GLN54 | 0.86 | 1.00 |
| LEU55 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R53HA | 1.00 |
| Q54HB2 | 1.00 |
| Q54HB3 | 1.00 |
| Q54HG2 | 1.00 |
| Q54HG3 | 1.00 |
| Q54H | 1.00 |
| Q54HA | 1.00 |
| L55H | 1.00 |
| L55HA | 1.00 |

NOESY contacts detailed probability

3.54 GLN(54)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG53 | HA | 1.00 | 0.005 | 1.00 | 0.16 |
| ARG53 | HB3 | 0.79 | 0.000 | 1.00 | 0.12 |
| ARG53 | H | 0.90 | 0.010 | 1.00 | -125114.00 |
| GLN54 | HA | 1.00 | 0.337 | 0.00 | 0.00 |
| GLN54 | HB2 | 1.00 | 0.002 | 1.00 | 1.17 |
| GLN54 | HB3 | 1.00 | 0.002 | 1.00 | 1.17 |
| GLN54 | HG2 | 1.00 | 0.002 | 1.00 | 0.82 |
| GLN54 | HG3 | 1.00 | 0.002 | 1.00 | 0.67 |
| GLN54 | H | 1.00 | 0.002 | 1.00 | -1374715.00 |
| GLN54 | HE21 | 0.94 | 0.016 | 1.00 | -147438.00 |
| LEU55 | HA | 1.00 | 0.001 | 1.00 | 36.36 |
| LEU55 | H | 1.00 | 0.018 | 1.00 | -1352144.00 |

3.54.7 Detailed Probabilities of GLN54HB2:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN54 | 0.75 | 1.00 |
| LEU55 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q54HA | 1.00 |
| Q54HB3 | 1.00 |
| Q54HG2 | 1.00 |
| Q54HG3 | 1.00 |
| Q54H | 1.00 |
| Q54HE21 | 1.00 |
| Q54HE22 | 1.00 |
| Q54HB2 | 1.00 |
| L55H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN54 | HA | 1.00 | 0.013 | 1.00 | 2.76 |
| GLN54 | HB2 | 1.00 | 0.471 | 0.00 | 0.00 |
| GLN54 | HB3 | 1.00 | 0.472 | 0.00 | 0.00 |
| GLN54 | HG2 | 1.00 | 0.005 | 1.00 | 1.90 |
| GLN54 | HG3 | 1.00 | 0.003 | 1.00 | 1.86 |
| GLN54 | H | 1.00 | 0.004 | 1.00 | -3003286.00 |
| GLN54 | HE21 | 1.00 | 0.013 | 1.00 | -332928.00 |
| GLN54 | HE22 | 1.00 | 0.013 | 1.00 | -238373.00 |
| LEU55 | H | 1.00 | 0.005 | 1.00 | -1308744.00 |

3.54.8 Detailed Probabilities of GLN54HB3:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN54 | 0.75 | 1.00 |
| LEU55 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q54HA | 1.00 |
| Q54HB2 | 1.00 |
| Q54HG2 | 1.00 |
| Q54HG3 | 1.00 |
| Q54H | 1.00 |
| Q54HE21 | 1.00 |
| Q54HE22 | 1.00 |
| Q54HB3 | 1.00 |
| L55H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN54 | HA | 1.00 | 0.013 | 1.00 | 2.76 |
| GLN54 | HB2 | 1.00 | 0.471 | 0.00 | 0.00 |
| GLN54 | HB3 | 1.00 | 0.472 | 0.00 | 0.00 |
| GLN54 | HG2 | 1.00 | 0.005 | 1.00 | 1.90 |
| GLN54 | HG3 | 1.00 | 0.003 | 1.00 | 1.86 |
| GLN54 | H | 1.00 | 0.004 | 1.00 | -3003286.00 |
| GLN54 | HE21 | 1.00 | 0.013 | 1.00 | -332928.00 |
| GLN54 | HE22 | 1.00 | 0.013 | 1.00 | -238373.00 |
| LEU55 | H | 1.00 | 0.005 | 1.00 | -1308744.00 |

3.54.9 Detailed Probabilities of GLN54HG2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN54 | 1.00 | 1.00 |
| LEU55 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q54HA | 1.00 |
| Q54HB2 | 1.00 |
| Q54HB3 | 1.00 |
| Q54HG3 | 1.00 |
| Q54H | 1.00 |
| Q54HE21 | 1.00 |
| Q54HE22 | 1.00 |
| Q54HG2 | 1.00 |
| L55H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN54 | HA | 1.00 | 0.006 | 1.00 | 0.69 |
| GLN54 | HB2 | 1.00 | 0.009 | 1.00 | 0.91 |
| GLN54 | HB3 | 1.00 | 0.009 | 1.00 | 0.91 |
| GLN54 | HG2 | 1.00 | 0.005 | 1.00 | 12.43 |
| GLN54 | HG3 | 1.00 | 0.004 | 1.00 | 8.47 |
| GLN54 | H | 1.00 | 0.007 | 1.00 | -1247489.00 |
| GLN54 | HE21 | 1.00 | 0.005 | 1.00 | -515743.00 |
| GLN54 | HE22 | 1.00 | 0.005 | 1.00 | -344080.00 |
| LEU55 | H | 0.98 | 0.008 | 1.00 | -204650.00 |

3.54.10 Detailed Probabilities of GLN54HG3:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN54 | 1.00 | 1.00 |
| LEU55 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q54HA | 1.00 |
| Q54HB2 | 1.00 |
| Q54HB3 | 1.00 |
| Q54HG2 | 1.00 |
| Q54H | 1.00 |
| Q54HE21 | 1.00 |
| Q54HE22 | 1.00 |
| Q54HG3 | 1.00 |
| L55H | 0.97 |

NOESY contacts detailed probability

3.54 GLN(54)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN54 | HA | 1.00 | 0.004 | 1.00 | 0.44 |
| GLN54 | HB2 | 1.00 | 0.000 | 1.00 | 0.94 |
| GLN54 | HB3 | 1.00 | 0.000 | 1.00 | 0.94 |
| GLN54 | HG2 | 1.00 | 0.000 | 1.00 | 9.00 |
| GLN54 | HG3 | 1.00 | 0.002 | 1.00 | 11.87 |
| GLN54 | H | 1.00 | 0.000 | 1.00 | -1226057.00 |
| GLN54 | HE21 | 1.00 | 0.002 | 1.00 | -743910.00 |
| GLN54 | HE22 | 1.00 | 0.002 | 1.00 | -436550.00 |
| LEU55 | H | 0.97 | 0.002 | 1.00 | -168818.00 |

3.54.11 Detailed Probabilities of GLN54H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG53 | 1.00 | 1.00 |
| GLN54 | 1.00 | 1.00 |
| LEU55 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R53H | 1.00 |
| R53HB2 | 1.00 |
| R53HG2 | 0.97 |
| R53HG3 | 0.96 |
| R53HA | 1.00 |
| R53HB3 | 1.00 |
| Q54HA | 1.00 |
| Q54HB2 | 1.00 |
| Q54HB3 | 1.00 |
| Q54HG2 | 1.00 |
| Q54HG3 | 1.00 |
| Q54H | 1.00 |
| L55H | 1.00 |

NOESY contacts detailed probability

3.54 GLN(54)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG53 | HA | 1.00 | 0.003 | 1.00 | 0.22 |
| ARG53 | HB2 | 1.00 | 0.004 | 1.00 | 0.38 |
| ARG53 | HB3 | 1.00 | 0.001 | 1.00 | 0.39 |
| ARG53 | HG2 | 0.97 | 0.007 | 1.00 | 0.18 |
| ARG53 | HG3 | 0.96 | 0.000 | 1.00 | 0.19 |
| ARG53 | H | 1.00 | 0.000 | 1.00 | -1145175.00 |
| ARG53 | HD2 | 0.54 | 0.004 | 1.00 | 0.10 |
| ARG53 | HD3 | 0.58 | 0.004 | 1.00 | 0.10 |
| GLN54 | HA | 1.00 | 0.003 | 1.00 | 0.73 |
| GLN54 | HB2 | 1.00 | 0.003 | 1.00 | 0.90 |
| GLN54 | HB3 | 1.00 | 0.003 | 1.00 | 0.90 |
| GLN54 | HG2 | 1.00 | 0.002 | 1.00 | 0.73 |
| GLN54 | HG3 | 1.00 | 0.001 | 1.00 | 0.72 |
| GLN54 | H | 1.00 | 0.002 | 1.00 | -14186829.00 |
| LEU55 | H | 1.00 | 0.001 | 1.00 | -1558464.00 |

3.54.12 Detailed Probabilities of GLN54HE21:

Overall probability: 0.333

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN54 | 0.33 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q54HB2 | 1.00 |
| Q54HB3 | 1.00 |
| Q54HG2 | 1.00 |
| Q54HG3 | 1.00 |
| Q54HE22 | 1.00 |
| Q54HE21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN54 | HB2 | 1.00 | 0.076 | 0.00 | 0.00 |
| GLN54 | HB3 | 1.00 | 0.076 | 0.00 | 0.00 |
| GLN54 | HG2 | 1.00 | 0.071 | 0.00 | 0.00 |
| GLN54 | HG3 | 1.00 | 0.074 | 0.00 | 0.00 |
| GLN54 | HE21 | 1.00 | 0.004 | 1.00 | -22583980.00 |
| GLN54 | HE22 | 1.00 | 0.004 | 1.00 | -16100147.00 |

3.54.13 Detailed Probabilities of GLN54HE22:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN54 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q54HB2 | 1.00 |
| Q54HB3 | 1.00 |
| Q54HG2 | 1.00 |
| Q54HG3 | 1.00 |
| Q54HE21 | 1.00 |
| Q54HE22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN54 | HB2 | 1.00 | 0.055 | 0.00 | 0.00 |
| GLN54 | HB3 | 1.00 | 0.055 | 0.00 | 0.00 |
| GLN54 | HG2 | 1.00 | 0.000 | 1.00 | 0.11 |
| GLN54 | HG3 | 1.00 | 0.004 | 1.00 | 0.11 |
| GLN54 | HE21 | 1.00 | 0.001 | 1.00 | -14435378.00 |
| GLN54 | HE22 | 1.00 | 0.001 | 1.00 | -22984860.00 |

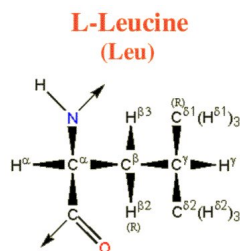
3.55 LEU(55)

Figure 45: Image from the BMRB

Residue probability: 0.797

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 177.473 | 177.056 | 1.929 | 0.000 | 0.000 |
| CA 3.55.1 | 57.831 | 55.735 | 3.802 | 0.501 | 1.000 |
| CB 3.55.2 | 41.811 | 42.389 | 3.750 | 1.000 | 1.000 |
| CG 3.55.3 | 27.193 | 26.892 | 3.086 | 0.750 | 1.000 |
| CD1 3.55.4 | 26.807 | 24.837 | 3.657 | 0.814 | 1.000 |
| CD2 3.55.5 | 24.046 | 24.201 | 3.117 | 0.714 | 1.000 |
| N 3.55.6 | 121.646 | 121.785 | 4.943 | 1.000 | 1.000 |
| HA 3.55.7 | 4.026 | 4.315 | 0.840 | 0.846 | 1.000 |
| HB2 3.55.8 | 1.870 | 1.601 | 0.373 | 0.750 | 1.000 |
| HB3 3.55.9 | 0.914 | 1.508 | 0.398 | 0.963 | 1.000 |
| HG 3.55.10 | 1.695 | 1.510 | 0.340 | 1.000 | 1.000 |
| HD1 3.55.11 | 0.643 | 0.739 | 0.294 | 0.668 | 1.000 |
| HD2 3.55.12 | 0.717 | 0.727 | 0.421 | 0.429 | 1.000 |
| H 3.55.13 | 8.106 | 8.237 | 0.647 | 0.933 | 1.000 |

3.55.1 Detailed Probabilities of LEU55CA:

Overall probability: 0.501

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN54 | 1.00 | 1.00 |
| LEU55 | 0.57 | 1.00 |
| PHE56 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q54HA | 1.00 |
| L55HB2 | 1.00 |
| L55HB3 | 1.00 |
| L55HG | 1.00 |
| L55HD11 | 0.99 |
| L55HD21 | 0.99 |
| L55H | 1.00 |
| L55HA | 1.00 |
| F56HA | 1.00 |
| F56H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN54 | HA | 1.00 | 0.001 | 1.00 | 36.36 |
| LEU55 | HA | 1.00 | 0.026 | 1.00 | 36.36 |
| LEU55 | HB2 | 1.00 | 0.128 | 0.00 | 0.00 |
| LEU55 | HB3 | 1.00 | 0.006 | 1.00 | 0.89 |
| LEU55 | HG | 1.00 | 0.001 | 1.00 | 1.04 |
| LEU55 | HD11 | 0.99 | 0.083 | 0.01 | 0.00 |
| LEU55 | HD21 | 0.99 | 0.009 | 1.00 | 1.82 |
| LEU55 | H | 1.00 | 0.169 | 0.00 | 0.00 |
| PHE56 | HA | 1.00 | 0.094 | 0.00 | 0.00 |
| PHE56 | H | 1.00 | 0.403 | 0.00 | 0.00 |

3.55.2 Detailed Probabilities of LEU55CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU55 | 1.00 | 1.00 |
| PHE56 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L55HA | 1.00 |
| L55HB2 | 1.00 |
| L55HG | 1.00 |
| L55HD11 | 1.00 |
| L55HD21 | 1.00 |
| L55H | 1.00 |
| L55HB3 | 1.00 |
| F56H | 1.00 |

NOESY contacts detailed probability

3.55 LEU(55)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU55 | HA | 1.00 | 0.002 | 1.00 | 0.28 |
| LEU55 | HB2 | 1.00 | 0.000 | 1.00 | 0.93 |
| LEU55 | HB3 | 1.00 | 0.000 | 1.00 | 1.35 |
| LEU55 | HG | 1.00 | 0.000 | 1.00 | 0.25 |
| LEU55 | HD11 | 1.00 | 0.012 | 1.00 | 0.46 |
| LEU55 | HD21 | 1.00 | 0.001 | 1.00 | 0.49 |
| LEU55 | H | 1.00 | 0.004 | 1.00 | 0.28 |
| PHE56 | H | 1.00 | 0.002 | 1.00 | 0.09 |

3.55.3 Detailed Probabilities of LEU55CG:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU55 | 0.71 | 1.00 |
| PHE56 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L55HA | 1.00 |
| L55HB2 | 1.00 |
| L55HB3 | 1.00 |
| L55HD11 | 1.00 |
| L55HD21 | 1.00 |
| L55H | 1.00 |
| L55HG | 1.00 |
| F56H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU55 | HA | 1.00 | 0.015 | 1.00 | 0.46 |
| LEU55 | HB2 | 1.00 | 0.065 | 0.00 | 0.00 |
| LEU55 | HB3 | 1.00 | 0.002 | 1.00 | 3.90 |
| LEU55 | HG | 1.00 | 0.015 | 1.00 | 27.01 |
| LEU55 | HD11 | 1.00 | 0.003 | 1.00 | 1.19 |
| LEU55 | HD21 | 1.00 | 0.077 | 0.00 | 0.00 |
| LEU55 | H | 1.00 | 0.007 | 1.00 | 0.40 |
| PHE56 | H | 0.98 | 0.020 | 1.00 | 0.12 |

3.55.4 Detailed Probabilities of LEU55CD1:

Overall probability: 0.814

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU55 | 0.81 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L55HA | 0.99 |
| L55HB2 | 1.00 |
| L55HB3 | 1.00 |
| L55HG | 1.00 |
| L55HD12 | 1.00 |
| L55HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU55 | HA | 0.99 | 0.007 | 1.00 | 0.20 |
| LEU55 | HB2 | 1.00 | 0.001 | 1.00 | 0.75 |
| LEU55 | HB3 | 1.00 | 0.033 | 0.70 | 0.00 |
| LEU55 | HG | 1.00 | 0.006 | 1.00 | 1.39 |
| LEU55 | HD11 | 1.00 | 0.001 | 1.00 | 22.31 |
| LEU55 | HD21 | 1.00 | 0.075 | 0.00 | 0.00 |
| LEU55 | H | 0.86 | 0.006 | 1.00 | 0.42 |

3.55.5 Detailed Probabilities of LEU55CD2:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU55 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L55HA | 0.99 |
| L55HB2 | 1.00 |
| L55HB3 | 1.00 |
| L55HG | 1.00 |
| L55HD11 | 1.00 |
| L55HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU55 | HA | 0.99 | 0.001 | 1.00 | 1.87 |
| LEU55 | HB2 | 1.00 | 0.007 | 1.00 | 0.80 |
| LEU55 | HB3 | 1.00 | 0.003 | 1.00 | 1.98 |
| LEU55 | HG | 1.00 | 0.004 | 1.00 | 1.49 |
| LEU55 | HD11 | 1.00 | 0.142 | 0.00 | 0.00 |
| LEU55 | HD21 | 1.00 | 0.200 | 0.00 | 0.00 |
| LEU55 | H | 0.85 | 0.012 | 1.00 | 0.45 |

3.55.6 Detailed Probabilities of LEU55N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN54 | 1.00 | 1.00 |
| LEU55 | 1.00 | 1.00 |
| PHE56 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Q54HG3 | 0.97 |
| Q54HB3 | 1.00 |
| Q54HA | 1.00 |
| Q54H | 1.00 |
| Q54HG2 | 0.98 |
| Q54HB2 | 1.00 |
| L55HA | 1.00 |
| L55HB2 | 1.00 |
| L55HB3 | 1.00 |
| L55HG | 1.00 |
| L55H | 1.00 |
| F56H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN54 | HA | 1.00 | 0.018 | 1.00 | -1352144.00 |
| GLN54 | HB2 | 1.00 | 0.004 | 1.00 | -1308744.00 |
| GLN54 | HB3 | 1.00 | 0.005 | 1.00 | -1308744.00 |
| GLN54 | HG2 | 0.98 | 0.008 | 1.00 | -204650.00 |
| GLN54 | HG3 | 0.97 | 0.002 | 1.00 | -168818.00 |
| GLN54 | H | 1.00 | 0.001 | 1.00 | -1558464.00 |
| LEU55 | HA | 1.00 | 0.007 | 1.00 | -1352144.00 |
| LEU55 | HB2 | 1.00 | 0.000 | 1.00 | -1666195.00 |
| LEU55 | HB3 | 1.00 | 0.000 | 1.00 | -1228582.00 |
| LEU55 | HG | 1.00 | 0.004 | 1.00 | -1797062.00 |
| LEU55 | H | 1.00 | 0.006 | 1.00 | -13248205.00 |
| LEU55 | HD21 | 0.87 | 0.022 | 1.00 | -966498.00 |
| PHE56 | H | 1.00 | 0.000 | 1.00 | -1281504.00 |
| PHE56 | HB2 | 0.58 | 0.003 | 1.00 | -118494.00 |

3.55.7 Detailed Probabilities of LEU55HA:

Overall probability: 0.846

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN54 | 0.75 | 1.00 |
| LEU55 | 1.00 | 1.00 |
| PHE56 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| Q54HA | 1.00 |
| L55HB2 | 1.00 |
| L55HB3 | 1.00 |
| L55HG | 1.00 |
| L55HD11 | 0.99 |
| L55HD21 | 0.99 |
| L55H | 1.00 |
| L55HA | 1.00 |
| F56HA | 1.00 |
| F56H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN54 | HA | 1.00 | 0.362 | 0.00 | 0.00 |
| GLN54 | HB2 | 0.72 | 0.027 | 1.00 | 1.17 |
| GLN54 | HB3 | 0.87 | 0.027 | 1.00 | 1.17 |
| GLN54 | H | 0.94 | 0.027 | 1.00 | -1374715.00 |
| LEU55 | HA | 1.00 | 0.026 | 1.00 | 36.36 |
| LEU55 | HB2 | 1.00 | 0.001 | 1.00 | 0.23 |
| LEU55 | HB3 | 1.00 | 0.002 | 1.00 | 0.28 |
| LEU55 | HG | 1.00 | 0.015 | 1.00 | 0.46 |
| LEU55 | HD11 | 0.99 | 0.007 | 1.00 | 0.20 |
| LEU55 | HD21 | 0.99 | 0.001 | 1.00 | 1.87 |
| LEU55 | H | 1.00 | 0.007 | 1.00 | -1352144.00 |
| PHE56 | HA | 1.00 | 0.082 | 0.00 | 0.00 |
| PHE56 | H | 1.00 | 0.011 | 1.00 | -586650.00 |

3.55.8 Detailed Probabilities of LEU55HB2:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU55 | 0.71 | 1.00 |
| PHE56 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L55HA | 1.00 |
| L55HB3 | 1.00 |
| L55HG | 1.00 |
| L55HD11 | 1.00 |
| L55HD21 | 1.00 |
| L55H | 1.00 |
| L55HB2 | 1.00 |
| F56H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU55 | HA | 1.00 | 0.128 | 0.00 | 0.00 |
| LEU55 | HB2 | 1.00 | 0.001 | 1.00 | 0.96 |
| LEU55 | HB3 | 1.00 | 0.000 | 1.00 | 0.93 |
| LEU55 | HG | 1.00 | 0.065 | 0.00 | 0.00 |
| LEU55 | HD11 | 1.00 | 0.001 | 1.00 | 0.75 |
| LEU55 | HD21 | 1.00 | 0.007 | 1.00 | 0.80 |
| LEU55 | H | 1.00 | 0.000 | 1.00 | -1666195.00 |
| PHE56 | H | 1.00 | 0.003 | 1.00 | -820025.00 |

3.55.9 Detailed Probabilities of LEU55HB3:

Overall probability: 0.963

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU55 | 0.96 | 1.00 |
| PHE56 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L55HA | 1.00 |
| L55HB2 | 1.00 |
| L55HG | 1.00 |
| L55HD11 | 1.00 |
| L55HD21 | 1.00 |
| L55H | 1.00 |
| L55HB3 | 1.00 |
| F56H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU55 | HA | 1.00 | 0.006 | 1.00 | 0.89 |
| LEU55 | HB2 | 1.00 | 0.000 | 1.00 | 1.05 |
| LEU55 | HB3 | 1.00 | 0.000 | 1.00 | 1.35 |
| LEU55 | HG | 1.00 | 0.002 | 1.00 | 3.90 |
| LEU55 | HD11 | 1.00 | 0.033 | 0.70 | 0.00 |
| LEU55 | HD21 | 1.00 | 0.003 | 1.00 | 1.98 |
| LEU55 | H | 1.00 | 0.000 | 1.00 | -1228582.00 |
| PHE56 | H | 1.00 | 0.001 | 1.00 | -551773.00 |

3.55.10 Detailed Probabilities of LEU55HG:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU55 | 1.00 | 1.00 |
| PHE56 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L55HA | 1.00 |
| L55HB2 | 1.00 |
| L55HB3 | 1.00 |
| L55HD11 | 1.00 |
| L55HD21 | 1.00 |
| L55H | 1.00 |
| L55HG | 1.00 |
| F56H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU55 | HA | 1.00 | 0.001 | 1.00 | 1.04 |
| LEU55 | HB2 | 1.00 | 0.000 | 1.00 | 0.25 |
| LEU55 | HB3 | 1.00 | 0.000 | 1.00 | 0.25 |
| LEU55 | HG | 1.00 | 0.015 | 1.00 | 27.01 |
| LEU55 | HD11 | 1.00 | 0.006 | 1.00 | 1.39 |
| LEU55 | HD21 | 1.00 | 0.004 | 1.00 | 1.49 |
| LEU55 | H | 1.00 | 0.004 | 1.00 | -1797062.00 |
| PHE56 | H | 0.98 | 0.001 | 1.00 | -374811.00 |

3.55.11 Detailed Probabilities of LEU55HD11:

Overall probability: 0.668

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU55 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L55HA | 0.99 |
| L55HB2 | 1.00 |
| L55HB3 | 1.00 |
| L55HG | 1.00 |
| L55HD12 | 1.00 |
| L55HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU55 | HA | 0.99 | 0.083 | 0.01 | 0.00 |
| LEU55 | HB2 | 1.00 | 0.001 | 1.00 | 0.47 |
| LEU55 | HB3 | 1.00 | 0.012 | 1.00 | 0.46 |
| LEU55 | HG | 1.00 | 0.003 | 1.00 | 1.19 |
| LEU55 | HD11 | 1.00 | 0.001 | 1.00 | 22.31 |
| LEU55 | HD21 | 1.00 | 0.142 | 0.00 | 0.00 |

3.55.12 Detailed Probabilities of LEU55HD21:

Overall probability: 0.429

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU55 | 0.43 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L55HA | 0.99 |
| L55HB2 | 1.00 |
| L55HB3 | 1.00 |
| L55HG | 1.00 |
| L55HD11 | 1.00 |
| L55HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU55 | HA | 0.99 | 0.009 | 1.00 | 1.82 |
| LEU55 | HB2 | 1.00 | 0.073 | 0.00 | 0.00 |
| LEU55 | HB3 | 1.00 | 0.001 | 1.00 | 0.49 |
| LEU55 | HG | 1.00 | 0.077 | 0.00 | 0.00 |
| LEU55 | HD11 | 1.00 | 0.075 | 0.00 | 0.00 |
| LEU55 | HD21 | 1.00 | 0.200 | 0.00 | 0.00 |
| LEU55 | H | 0.85 | 0.022 | 1.00 | -966498.00 |

3.55.13 Detailed Probabilities of LEU55H:

Overall probability: 0.933

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLN54 | 1.00 | 1.00 |
| LEU55 | 0.86 | 1.00 |
| PHE56 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Q54HG3 | 0.97 |
| Q54HB3 | 1.00 |
| Q54HA | 1.00 |
| Q54H | 1.00 |
| Q54HG2 | 0.98 |
| Q54HB2 | 1.00 |
| L55HA | 1.00 |
| L55HB2 | 1.00 |
| L55HB3 | 1.00 |
| L55HG | 1.00 |
| L55H | 1.00 |
| F56H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLN54 | HA | 1.00 | 0.002 | 1.00 | 0.30 |
| GLN54 | HB2 | 1.00 | 0.006 | 1.00 | 0.41 |
| GLN54 | HB3 | 1.00 | 0.006 | 1.00 | 0.41 |
| GLN54 | HG2 | 0.98 | 0.000 | 1.00 | 0.13 |
| GLN54 | HG3 | 0.97 | 0.006 | 1.00 | 0.11 |
| GLN54 | H | 1.00 | 0.005 | 1.00 | -1668657.00 |
| LEU55 | HA | 1.00 | 0.169 | 0.00 | 0.00 |
| LEU55 | HB2 | 1.00 | 0.004 | 1.00 | 0.31 |
| LEU55 | HB3 | 1.00 | 0.004 | 1.00 | 0.28 |
| LEU55 | HG | 1.00 | 0.007 | 1.00 | 0.40 |
| LEU55 | H | 1.00 | 0.006 | 1.00 | -13248205.00 |
| LEU55 | HD11 | 0.88 | 0.006 | 1.00 | 0.42 |
| LEU55 | HD21 | 0.87 | 0.012 | 1.00 | 0.45 |
| PHE56 | H | 1.00 | 0.007 | 1.00 | -1647418.00 |
| PHE56 | HB2 | 0.58 | 0.012 | 1.00 | 0.06 |

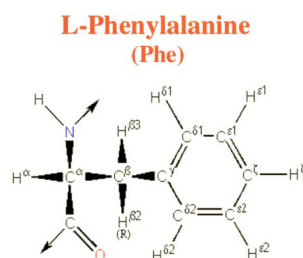
3.56 PHE(56)

Figure 46: Image from the BMRB

Residue probability: 0.884

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 176.433 | 175.508 | 2.010 | 0.000 | 0.000 |
| CA 3.56.1 | 61.477 | 58.245 | 3.808 | 0.801 | 1.000 |
| CB 3.56.2 | 38.913 | 40.078 | 3.616 | 0.967 | 1.000 |
| CD1 3.56.3 | 131.663 | 131.234 | 9.579 | 1.000 | 1.000 |
| CD2 3.56.4 | 131.801 | 131.352 | 9.581 | 1.000 | 1.000 |
| CE1 3.56.5 | 130.908 | 130.599 | 3.219 | 0.714 | 1.000 |
| CE2 3.56.6 | 131.004 | 130.633 | 2.839 | 0.572 | 1.000 |
| CZ 3.56.7 | 129.580 | 129.042 | 3.448 | 1.000 | 1.000 |
| N 3.56.8 | 113.667 | 120.315 | 4.931 | 1.000 | 1.000 |
| HA 3.56.9 | 4.107 | 4.625 | 1.237 | 0.800 | 1.000 |
| HB2 3.56.10 | 3.197 | 2.980 | 0.399 | 0.778 | 1.000 |
| HB3 3.56.11 | 2.793 | 2.916 | 0.434 | 1.000 | 1.000 |
| HD1 3.56.12 | 7.197 | 7.037 | 0.347 | 1.000 | 1.000 |
| HD2 3.56.13 | 7.197 | 7.022 | 0.417 | 1.000 | 1.000 |
| HE1 3.56.14 | 7.002 | 7.046 | 0.417 | 0.750 | 1.000 |
| HE2 3.56.15 | 7.002 | 7.043 | 0.400 | 0.714 | 1.000 |
| HZ 3.56.16 | 7.198 | 6.984 | 1.598 | 1.000 | 1.000 |
| H 3.56.17 | 7.872 | 8.375 | 0.710 | 0.929 | 1.000 |

3.56.1 Detailed Probabilities of PHE56CA:

Overall probability: 0.801

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU55 | 0.45 | 1.00 |
| PHE56 | 1.00 | 1.00 |
| ARG57 | 0.45 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L55HA | 1.00 |
| F56HB2 | 1.00 |
| F56HB3 | 1.00 |
| F56HD1 | 1.00 |
| F56HD2 | 1.00 |
| F56H | 1.00 |
| F56HA | 1.00 |
| R57H | 1.00 |
| R57HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU55 | HA | 1.00 | 0.082 | 0.00 | 0.00 |
| LEU55 | HB3 | 0.91 | 0.031 | 0.91 | 0.00 |
| PHE56 | HA | 1.00 | 0.001 | 1.00 | 7.21 |
| PHE56 | HB2 | 1.00 | 0.001 | 1.00 | 0.71 |
| PHE56 | HB3 | 1.00 | 0.002 | 1.00 | 0.45 |
| PHE56 | HD1 | 1.00 | 0.004 | 1.00 | 1.01 |
| PHE56 | HD2 | 1.00 | 0.004 | 1.00 | 1.01 |
| PHE56 | H | 1.00 | 0.000 | 1.00 | 0.58 |
| PHE56 | HE1 | 0.74 | 0.011 | 1.00 | 0.15 |
| ARG57 | HA | 1.00 | 0.103 | 0.00 | 0.00 |
| ARG57 | H | 1.00 | 0.031 | 0.90 | 0.00 |

3.56.2 Detailed Probabilities of PHE56CB:

Overall probability: 0.967

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE56 | 1.00 | 1.00 |
| ARG57 | 0.70 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F56HA | 1.00 |
| F56HB2 | 1.00 |
| F56HD1 | 1.00 |
| F56HD2 | 1.00 |
| F56HE2 | 1.00 |
| F56H | 1.00 |
| F56HB3 | 1.00 |
| R57H | 1.00 |

NOESY contacts detailed probability

3.56 PHE(56)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE56 | HA | 1.00 | 0.003 | 1.00 | 0.36 |
| PHE56 | HB2 | 1.00 | 0.001 | 1.00 | 1.55 |
| PHE56 | HB3 | 1.00 | 0.002 | 1.00 | 1.49 |
| PHE56 | HD1 | 1.00 | 0.002 | 1.00 | 0.57 |
| PHE56 | HD2 | 1.00 | 0.002 | 1.00 | 0.57 |
| PHE56 | HE2 | 1.00 | 0.013 | 1.00 | 0.08 |
| PHE56 | H | 1.00 | 0.002 | 1.00 | 0.55 |
| PHE56 | HE1 | 0.89 | 0.013 | 1.00 | 0.08 |
| ARG57 | H | 1.00 | 0.033 | 0.70 | 0.00 |

3.56.3 Detailed Probabilities of PHE56CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE56 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F56HA | 1.00 |
| F56HB2 | 1.00 |
| F56HB3 | 1.00 |
| F56HD2 | 1.00 |
| F56HE1 | 1.00 |
| F56HE2 | 1.00 |
| F56HZ | 1.00 |
| F56H | 1.00 |
| F56HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE56 | HA | 1.00 | 0.001 | 1.00 | 0.26 |
| PHE56 | HB2 | 1.00 | 0.001 | 1.00 | 0.23 |
| PHE56 | HB3 | 1.00 | 0.001 | 1.00 | 0.97 |
| PHE56 | HD1 | 1.00 | 0.007 | 1.00 | 41.74 |
| PHE56 | HD2 | 1.00 | 0.007 | 1.00 | 41.74 |
| PHE56 | HE1 | 1.00 | 0.004 | 1.00 | 0.88 |
| PHE56 | HE2 | 1.00 | 0.004 | 1.00 | 0.88 |
| PHE56 | HZ | 1.00 | 0.008 | 1.00 | 41.74 |
| PHE56 | H | 1.00 | 0.003 | 1.00 | 0.14 |

3.56.4 Detailed Probabilities of PHE56CD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE56 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F56HA | 1.00 |
| F56HB2 | 1.00 |
| F56HB3 | 1.00 |
| F56HD1 | 1.00 |
| F56HE1 | 1.00 |
| F56HE2 | 1.00 |
| F56HZ | 1.00 |
| F56H | 0.99 |
| F56HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE56 | HA | 1.00 | 0.001 | 1.00 | 0.26 |
| PHE56 | HB2 | 1.00 | 0.001 | 1.00 | 0.23 |
| PHE56 | HB3 | 1.00 | 0.001 | 1.00 | 0.97 |
| PHE56 | HD1 | 1.00 | 0.007 | 1.00 | 41.74 |
| PHE56 | HD2 | 1.00 | 0.007 | 1.00 | 41.74 |
| PHE56 | HE1 | 1.00 | 0.004 | 1.00 | 0.88 |
| PHE56 | HE2 | 1.00 | 0.004 | 1.00 | 0.88 |
| PHE56 | HZ | 1.00 | 0.008 | 1.00 | 41.74 |
| PHE56 | H | 0.99 | 0.003 | 1.00 | 0.14 |

3.56.5 Detailed Probabilities of PHE56CE1:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE56 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F56HD1 | 1.00 |
| F56HD2 | 1.00 |
| F56HE2 | 1.00 |
| F56HZ | 1.00 |
| F56HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE56 | HD1 | 1.00 | 0.001 | 1.00 | 0.84 |
| PHE56 | HD2 | 1.00 | 0.001 | 1.00 | 0.84 |
| PHE56 | HE1 | 1.00 | 0.108 | 0.00 | 0.00 |
| PHE56 | HE2 | 1.00 | 0.108 | 0.00 | 0.00 |
| PHE56 | HZ | 1.00 | 0.002 | 1.00 | 0.84 |
| PHE56 | HA | 0.74 | 0.002 | 1.00 | 0.14 |
| PHE56 | HB3 | 0.89 | 0.004 | 1.00 | 0.15 |

3.56.6 Detailed Probabilities of PHE56CE2:

Overall probability: 0.572

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE56 | 0.57 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F56HB2 | 1.00 |
| F56HB3 | 1.00 |
| F56HD1 | 1.00 |
| F56HD2 | 1.00 |
| F56HE1 | 1.00 |
| F56HZ | 1.00 |
| F56HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE56 | HB2 | 1.00 | 0.323 | 0.00 | 0.00 |
| PHE56 | HB3 | 1.00 | 0.004 | 1.00 | 0.15 |
| PHE56 | HD1 | 1.00 | 0.001 | 1.00 | 0.84 |
| PHE56 | HD2 | 1.00 | 0.001 | 1.00 | 0.84 |
| PHE56 | HE1 | 1.00 | 0.108 | 0.00 | 0.00 |
| PHE56 | HE2 | 1.00 | 0.108 | 0.00 | 0.00 |
| PHE56 | HZ | 1.00 | 0.002 | 1.00 | 0.84 |

3.56.7 Detailed Probabilities of PHE56CZ:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE56 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F56HD1 | 1.00 |
| F56HD2 | 1.00 |
| F56HE1 | 1.00 |
| F56HE2 | 1.00 |
| F56HZ | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE56 | HD1 | 1.00 | 0.007 | 1.00 | 27.60 |
| PHE56 | HD2 | 1.00 | 0.007 | 1.00 | 27.60 |
| PHE56 | HE1 | 1.00 | 0.000 | 1.00 | 0.15 |
| PHE56 | HE2 | 1.00 | 0.000 | 1.00 | 0.15 |
| PHE56 | HZ | 1.00 | 0.008 | 1.00 | 27.60 |

3.56.8 Detailed Probabilities of PHE56N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU55 | 1.00 | 1.00 |
| PHE56 | 1.00 | 1.00 |
| ARG57 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L55HA | 1.00 |
| L55HG | 0.98 |
| L55HB2 | 1.00 |
| L55HB3 | 1.00 |
| L55H | 1.00 |
| F56HA | 1.00 |
| F56HB2 | 1.00 |
| F56HB3 | 1.00 |
| F56HD1 | 1.00 |
| F56HD2 | 0.99 |
| F56H | 1.00 |
| R57H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU55 | HA | 1.00 | 0.011 | 1.00 | -586650.00 |
| LEU55 | HB2 | 1.00 | 0.003 | 1.00 | -820025.00 |
| LEU55 | HB3 | 1.00 | 0.001 | 1.00 | -551773.00 |
| LEU55 | HG | 0.98 | 0.001 | 1.00 | -374811.00 |
| LEU55 | H | 1.00 | 0.007 | 1.00 | -1647418.00 |
| LEU55 | HD11 | 0.55 | 0.004 | 1.00 | -237543.00 |
| LEU55 | HD21 | 0.61 | 0.010 | 1.00 | -320805.00 |
| PHE56 | HA | 1.00 | 0.003 | 1.00 | -1216523.00 |
| PHE56 | HB2 | 1.00 | 0.002 | 1.00 | -1360738.00 |
| PHE56 | HB3 | 1.00 | 0.001 | 1.00 | -2136577.00 |
| PHE56 | HD1 | 1.00 | 0.019 | 1.00 | -2021385.00 |
| PHE56 | HD2 | 0.99 | 0.019 | 1.00 | -2021385.00 |
| PHE56 | H | 1.00 | 0.001 | 1.00 | -12832204.00 |
| ARG57 | H | 1.00 | 0.016 | 1.00 | -2021385.00 |
| ARG57 | HA | 0.90 | 0.020 | 1.00 | -165719.00 |

3.56.9 Detailed Probabilities of PHE56HA:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU55 | 0.00 | 1.00 |
| PHE56 | 1.00 | 1.00 |
| ARG57 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L55HA | 1.00 |
| F56HB2 | 1.00 |
| F56HB3 | 1.00 |
| F56HD1 | 1.00 |
| F56HD2 | 1.00 |
| F56H | 1.00 |
| F56HA | 1.00 |
| R57H | 1.00 |
| R57HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU55 | HA | 1.00 | 0.094 | 0.00 | 0.00 |
| PHE56 | HA | 1.00 | 0.001 | 1.00 | 7.21 |
| PHE56 | HB2 | 1.00 | 0.004 | 1.00 | 0.61 |
| PHE56 | HB3 | 1.00 | 0.003 | 1.00 | 0.36 |
| PHE56 | HD1 | 1.00 | 0.001 | 1.00 | 0.26 |
| PHE56 | HD2 | 1.00 | 0.001 | 1.00 | 0.26 |
| PHE56 | H | 1.00 | 0.003 | 1.00 | -1216523.00 |
| PHE56 | HE1 | 0.74 | 0.002 | 1.00 | 0.14 |
| ARG57 | HA | 1.00 | 0.094 | 0.00 | 0.00 |
| ARG57 | H | 1.00 | 0.002 | 1.00 | -650043.00 |

3.56.10 Detailed Probabilities of PHE56HB2:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE56 | 0.71 | 1.00 |
| ARG57 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F56HA | 1.00 |
| F56HB3 | 1.00 |
| F56HD1 | 1.00 |
| F56HD2 | 1.00 |
| F56HE2 | 1.00 |
| F56H | 1.00 |
| F56HB2 | 1.00 |
| R57H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE56 | HA | 1.00 | 0.001 | 1.00 | 0.71 |
| PHE56 | HB2 | 1.00 | 0.407 | 0.00 | 0.00 |
| PHE56 | HB3 | 1.00 | 0.001 | 1.00 | 1.55 |
| PHE56 | HD1 | 1.00 | 0.001 | 1.00 | 0.23 |
| PHE56 | HD2 | 1.00 | 0.001 | 1.00 | 0.23 |
| PHE56 | HE2 | 1.00 | 0.323 | 0.00 | 0.00 |
| PHE56 | H | 1.00 | 0.002 | 1.00 | -1360738.00 |
| ARG57 | H | 1.00 | 0.003 | 1.00 | -761685.00 |
| ARG57 | HA | 0.64 | 0.010 | 1.00 | 0.43 |

3.56.11 Detailed Probabilities of PHE56HB3:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE56 | 1.00 | 1.00 |
| ARG57 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F56HA | 1.00 |
| F56HB2 | 1.00 |
| F56HD1 | 1.00 |
| F56HD2 | 1.00 |
| F56HE2 | 1.00 |
| F56H | 1.00 |
| F56HB3 | 1.00 |
| R57H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE56 | HA | 1.00 | 0.002 | 1.00 | 0.45 |
| PHE56 | HB2 | 1.00 | 0.003 | 1.00 | 1.67 |
| PHE56 | HB3 | 1.00 | 0.002 | 1.00 | 1.49 |
| PHE56 | HD1 | 1.00 | 0.001 | 1.00 | 0.97 |
| PHE56 | HD2 | 1.00 | 0.001 | 1.00 | 0.97 |
| PHE56 | HE2 | 1.00 | 0.004 | 1.00 | 0.15 |
| PHE56 | H | 1.00 | 0.001 | 1.00 | -2136577.00 |
| PHE56 | HE1 | 0.89 | 0.004 | 1.00 | 0.15 |
| ARG57 | H | 1.00 | 0.002 | 1.00 | -356000.00 |

3.56.12 Detailed Probabilities of PHE56HD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE56 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F56HA | 1.00 |
| F56HB2 | 1.00 |
| F56HB3 | 1.00 |
| F56HD2 | 1.00 |
| F56HE1 | 1.00 |
| F56HE2 | 1.00 |
| F56HZ | 1.00 |
| F56H | 1.00 |
| F56HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE56 | HA | 1.00 | 0.004 | 1.00 | 1.01 |
| PHE56 | HB2 | 1.00 | 0.001 | 1.00 | 0.63 |
| PHE56 | HB3 | 1.00 | 0.002 | 1.00 | 0.57 |
| PHE56 | HD1 | 1.00 | 0.007 | 1.00 | 41.74 |
| PHE56 | HD2 | 1.00 | 0.007 | 1.00 | 41.74 |
| PHE56 | HE1 | 1.00 | 0.001 | 1.00 | 0.84 |
| PHE56 | HE2 | 1.00 | 0.001 | 1.00 | 0.84 |
| PHE56 | HZ | 1.00 | 0.007 | 1.00 | 27.60 |
| PHE56 | H | 1.00 | 0.019 | 1.00 | -2021385.00 |

3.56.13 Detailed Probabilities of PHE56HD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE56 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F56HA | 1.00 |
| F56HB2 | 1.00 |
| F56HB3 | 1.00 |
| F56HD1 | 1.00 |
| F56HE1 | 1.00 |
| F56HE2 | 1.00 |
| F56HZ | 1.00 |
| F56H | 0.99 |
| F56HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE56 | HA | 1.00 | 0.004 | 1.00 | 1.01 |
| PHE56 | HB2 | 1.00 | 0.001 | 1.00 | 0.63 |
| PHE56 | HB3 | 1.00 | 0.002 | 1.00 | 0.57 |
| PHE56 | HD1 | 1.00 | 0.007 | 1.00 | 41.74 |
| PHE56 | HD2 | 1.00 | 0.007 | 1.00 | 41.74 |
| PHE56 | HE1 | 1.00 | 0.001 | 1.00 | 0.84 |
| PHE56 | HE2 | 1.00 | 0.001 | 1.00 | 0.84 |
| PHE56 | HZ | 1.00 | 0.007 | 1.00 | 27.60 |
| PHE56 | H | 0.99 | 0.019 | 1.00 | -2021385.00 |

3.56.14 Detailed Probabilities of PHE56HE1:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE56 | 0.75 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F56HD1 | 1.00 |
| F56HD2 | 1.00 |
| F56HE2 | 1.00 |
| F56HZ | 1.00 |
| F56HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE56 | HD1 | 1.00 | 0.004 | 1.00 | 0.88 |
| PHE56 | HD2 | 1.00 | 0.004 | 1.00 | 0.88 |
| PHE56 | HE1 | 1.00 | 0.108 | 0.00 | 0.00 |
| PHE56 | HE2 | 1.00 | 0.108 | 0.00 | 0.00 |
| PHE56 | HZ | 1.00 | 0.000 | 1.00 | 0.15 |
| PHE56 | HA | 0.74 | 0.011 | 1.00 | 0.15 |
| PHE56 | HB2 | 0.90 | 0.005 | 1.00 | 0.09 |
| PHE56 | HB3 | 0.89 | 0.013 | 1.00 | 0.08 |

3.56.15 Detailed Probabilities of PHE56HE2:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE56 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F56HB2 | 1.00 |
| F56HB3 | 1.00 |
| F56HD1 | 1.00 |
| F56HD2 | 1.00 |
| F56HE1 | 1.00 |
| F56HZ | 1.00 |
| F56HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE56 | HB2 | 1.00 | 0.005 | 1.00 | 0.09 |
| PHE56 | HB3 | 1.00 | 0.013 | 1.00 | 0.08 |
| PHE56 | HD1 | 1.00 | 0.004 | 1.00 | 0.88 |
| PHE56 | HD2 | 1.00 | 0.004 | 1.00 | 0.88 |
| PHE56 | HE1 | 1.00 | 0.108 | 0.00 | 0.00 |
| PHE56 | HE2 | 1.00 | 0.108 | 0.00 | 0.00 |
| PHE56 | HZ | 1.00 | 0.000 | 1.00 | 0.15 |

3.56.16 Detailed Probabilities of PHE56HZ:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE56 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F56HD1 | 1.00 |
| F56HD2 | 1.00 |
| F56HE1 | 1.00 |
| F56HE2 | 1.00 |
| F56HZ | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE56 | HD1 | 1.00 | 0.008 | 1.00 | 41.74 |
| PHE56 | HD2 | 1.00 | 0.008 | 1.00 | 41.74 |
| PHE56 | HE1 | 1.00 | 0.002 | 1.00 | 0.84 |
| PHE56 | HE2 | 1.00 | 0.002 | 1.00 | 0.84 |
| PHE56 | HZ | 1.00 | 0.008 | 1.00 | 27.60 |

3.56.17 Detailed Probabilities of PHE56H:

Overall probability: 0.929

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU55 | 0.83 | 1.00 |
| PHE56 | 1.00 | 1.00 |
| ARG57 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L55HA | 1.00 |
| L55HG | 0.98 |
| L55HB2 | 1.00 |
| L55HB3 | 1.00 |
| L55H | 1.00 |
| F56HA | 1.00 |
| F56HB2 | 1.00 |
| F56HB3 | 1.00 |
| F56HD1 | 1.00 |
| F56HD2 | 0.99 |
| F56H | 1.00 |
| R57H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU55 | HA | 1.00 | 0.403 | 0.00 | 0.00 |
| LEU55 | HB2 | 1.00 | 0.008 | 1.00 | 0.13 |
| LEU55 | HB3 | 1.00 | 0.002 | 1.00 | 0.09 |
| LEU55 | HG | 0.98 | 0.020 | 1.00 | 0.12 |
| LEU55 | H | 1.00 | 0.000 | 1.00 | -1281504.00 |
| LEU55 | HD11 | 0.55 | 0.001 | 1.00 | 0.07 |
| PHE56 | HA | 1.00 | 0.000 | 1.00 | 0.58 |
| PHE56 | HB2 | 1.00 | 0.001 | 1.00 | 0.54 |
| PHE56 | HB3 | 1.00 | 0.002 | 1.00 | 0.55 |
| PHE56 | HD1 | 1.00 | 0.003 | 1.00 | 0.14 |
| PHE56 | HD2 | 0.99 | 0.003 | 1.00 | 0.14 |
| PHE56 | H | 1.00 | 0.001 | 1.00 | -12832204.00 |
| ARG57 | H | 1.00 | 0.003 | 1.00 | -1324723.00 |
| ARG57 | HA | 0.90 | 0.018 | 1.00 | 0.07 |

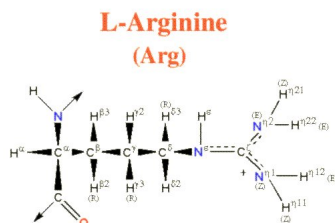


Figure 47: Image from the BMRB

Residue probability: 0.841
 Residue probability confidence: 0.867

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 175.964 | 176.453 | 2.303 | 0.000 | 0.000 |
| CA 3.57.1 | 57.175 | 56.803 | 3.326 | 0.769 | 1.000 |
| CB 3.57.2 | 29.511 | 30.892 | 2.424 | 0.938 | 0.889 |
| CG 3.57.3 | 27.310 | 27.247 | 1.538 | 0.912 | 0.800 |
| CD 3.57.4 | 43.100 | 43.189 | 1.415 | 1.000 | 0.667 |
| N 3.57.5 | 116.822 | 120.701 | 3.779 | 0.993 | 1.000 |
| NE | NA | - | - | 0.000 | 0.000 |
| NH1 | NA | - | - | 0.000 | 0.000 |
| NH2 | NA | - | - | 0.000 | 0.000 |
| HA 3.57.6 | 4.211 | 4.301 | 0.495 | 0.833 | 1.000 |
| HB2 3.57.7 | 1.898 | 1.793 | 0.292 | 0.538 | 0.889 |
| HB3 3.57.8 | 2.051 | 1.757 | 0.307 | 0.625 | 0.889 |
| HG2 3.57.9 | 1.713 | 1.559 | 0.294 | 1.000 | 0.800 |
| HG3 3.57.10 | 1.944 | 1.535 | 0.310 | 0.550 | 0.800 |
| HD 3.57.11 | 3.208 | 3.105 | 0.301 | 1.000 | 0.667 |
| H 3.57.12 | 7.232 | 8.248 | 0.623 | 0.938 | 1.000 |
| HE | NA | - | - | 0.000 | 0.000 |
| HH1 | NA | - | - | 0.000 | 0.000 |
| HH2 | NA | - | - | 0.000 | 0.000 |

3.57.1 Detailed Probabilities of ARG57CA:

Overall probability: 0.769
 Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE56 | 0.67 | 1.00 |
| ARG57 | 0.71 | 1.00 |
| ILE58 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F56HA | 1.00 |
| R57HB2 | 1.00 |
| R57HB3 | 1.00 |
| R57HG2 | 1.00 |
| R57HG3 | 1.00 |
| R57HD2 | 0.98 |
| R57H | 1.00 |
| R57HA | 1.00 |
| I58H | 1.00 |
| I58HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE56 | HA | 1.00 | 0.094 | 0.00 | 0.00 |
| PHE56 | HB2 | 0.64 | 0.010 | 1.00 | 0.43 |
| PHE56 | H | 0.90 | 0.018 | 1.00 | 0.07 |
| ARG57 | HA | 1.00 | 0.010 | 1.00 | 12.88 |
| ARG57 | HB2 | 1.00 | 0.156 | 0.00 | 0.00 |
| ARG57 | HB3 | 1.00 | 0.003 | 1.00 | 1.19 |
| ARG57 | HG2 | 1.00 | 0.009 | 1.00 | 1.09 |
| ARG57 | HG3 | 1.00 | 0.110 | 0.00 | 0.00 |
| ARG57 | HD2 | 0.98 | 0.001 | 1.00 | 0.43 |
| ARG57 | H | 1.00 | 0.003 | 1.00 | 0.72 |
| ILE58 | HA | 1.00 | 0.012 | 1.00 | 0.08 |
| ILE58 | H | 1.00 | 0.002 | 1.00 | 0.29 |
| ILE58 | HG12 | 0.51 | 0.002 | 1.00 | 1.09 |

3.57.2 Detailed Probabilities of ARG57CB:

Overall probability: 0.938

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG57 | 0.93 | 0.88 |
| ILE58 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R57HA | 1.00 |
| R57HB2 | 1.00 |
| R57HG2 | 1.00 |
| R57HG3 | 1.00 |
| R57HD2 | 1.00 |
| R57H | 1.00 |
| R57HE | 1.00 |
| R57HB3 | 1.00 |
| I58H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG57 | HA | 1.00 | 0.006 | 1.00 | 0.70 |
| ARG57 | HB2 | 1.00 | 0.011 | 1.00 | 3.56 |
| ARG57 | HB3 | 1.00 | 0.010 | 1.00 | 28.37 |
| ARG57 | HG2 | 1.00 | 0.007 | 1.00 | 1.04 |
| ARG57 | HG3 | 1.00 | 0.035 | 0.50 | 0.00 |
| ARG57 | HD2 | 1.00 | 0.005 | 1.00 | 0.46 |
| ARG57 | H | 1.00 | 0.002 | 1.00 | 0.51 |
| ILE58 | H | 1.00 | 0.002 | 1.00 | 0.09 |

3.57.3 Detailed Probabilities of ARG57CG:

Overall probability: 0.912

Overall confidence: 0.800

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG57 | 0.90 | 0.78 |
| ILE58 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R57HA | 1.00 |
| R57HB2 | 1.00 |
| R57HB3 | 1.00 |
| R57HG3 | 1.00 |
| R57HD2 | 1.00 |
| R57H | 1.00 |
| R57HE | 1.00 |
| R57HH11 | 1.00 |
| R57HG2 | 1.00 |
| I58H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG57 | HA | 1.00 | 0.003 | 1.00 | 0.85 |
| ARG57 | HB2 | 1.00 | 0.037 | 0.30 | 0.00 |
| ARG57 | HB3 | 1.00 | 0.005 | 1.00 | 1.36 |
| ARG57 | HG2 | 1.00 | 0.003 | 1.00 | 27.01 |
| ARG57 | HG3 | 1.00 | 0.009 | 1.00 | 5.96 |
| ARG57 | HD2 | 1.00 | 0.001 | 1.00 | 1.23 |
| ARG57 | H | 1.00 | 0.000 | 1.00 | 0.61 |
| ILE58 | H | 0.97 | 0.001 | 1.00 | 0.83 |

3.57.4 Detailed Probabilities of ARG57CD:

Overall probability: 1.000

Overall confidence: 0.667

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG57 | 1.00 | 0.67 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R57HA | 0.98 |
| R57HB2 | 1.00 |
| R57HB3 | 1.00 |
| R57HG2 | 1.00 |
| R57HG3 | 1.00 |
| R57HD3 | 1.00 |
| R57HE | 1.00 |
| R57HH11 | 1.00 |
| R57HH21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG57 | HA | 0.97 | 0.005 | 1.00 | 0.48 |
| ARG57 | HB2 | 1.00 | 0.030 | 1.00 | 0.00 |
| ARG57 | HB3 | 1.00 | 0.016 | 1.00 | 1.32 |
| ARG57 | HG2 | 1.00 | 0.002 | 1.00 | 1.77 |
| ARG57 | HG3 | 1.00 | 0.016 | 1.00 | 2.31 |
| ARG57 | HD2 | 1.00 | 0.014 | 1.00 | 52.97 |
| ARG57 | H | 0.86 | 0.019 | 1.00 | 0.62 |

3.57.5 Detailed Probabilities of ARG57N:

Overall probability: 0.993

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE56 | 1.00 | 1.00 |
| ARG57 | 0.99 | 1.00 |
| ILE58 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F56HB2 | 1.00 |
| F56H | 1.00 |
| F56HA | 1.00 |
| F56HB3 | 1.00 |
| R57HA | 1.00 |
| R57HB2 | 1.00 |
| R57HB3 | 1.00 |
| R57HG2 | 1.00 |
| R57HG3 | 1.00 |
| R57H | 1.00 |
| I58H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE56 | HA | 1.00 | 0.002 | 1.00 | -650043.00 |
| PHE56 | HB2 | 1.00 | 0.003 | 1.00 | -761685.00 |
| PHE56 | HB3 | 1.00 | 0.002 | 1.00 | -356000.00 |
| PHE56 | H | 1.00 | 0.003 | 1.00 | -1324723.00 |
| ARG57 | HA | 1.00 | 0.007 | 1.00 | -1803657.00 |
| ARG57 | HB2 | 1.00 | 0.015 | 1.00 | -3161249.00 |
| ARG57 | HB3 | 1.00 | 0.002 | 1.00 | -1554615.00 |
| ARG57 | HG2 | 1.00 | 0.005 | 1.00 | -1518405.00 |
| ARG57 | HG3 | 1.00 | 0.031 | 0.90 | 0.00 |
| ARG57 | H | 1.00 | 0.002 | 1.00 | -21018308.00 |
| ARG57 | HD2 | 0.87 | 0.008 | 1.00 | -761685.00 |
| ILE58 | H | 1.00 | 0.002 | 1.00 | -2502456.00 |
| ILE58 | HA | 0.93 | 0.014 | 1.00 | -197457.00 |
| ILE58 | HG13 | 0.55 | 0.019 | 1.00 | -342256.00 |

3.57.6 Detailed Probabilities of ARG57HA:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE56 | 0.50 | 1.00 |
| ARG57 | 0.86 | 1.00 |
| ILE58 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F56HA | 1.00 |
| R57HB2 | 1.00 |
| R57HB3 | 1.00 |
| R57HG2 | 1.00 |
| R57HG3 | 1.00 |
| R57HD2 | 0.98 |
| R57H | 1.00 |
| R57HA | 1.00 |
| I58H | 1.00 |
| I58HA | 1.00 |

NOESY contacts detailed probability

3.57 ARG(57)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE56 | HA | 1.00 | 0.103 | 0.00 | 0.00 |
| PHE56 | H | 0.90 | 0.020 | 1.00 | -165719.00 |
| ARG57 | HA | 1.00 | 0.010 | 1.00 | 12.88 |
| ARG57 | HB2 | 1.00 | 1.005 | 0.00 | 0.00 |
| ARG57 | HB3 | 1.00 | 0.006 | 1.00 | 0.70 |
| ARG57 | HG2 | 1.00 | 0.003 | 1.00 | 0.85 |
| ARG57 | HG3 | 1.00 | 0.008 | 1.00 | 0.59 |
| ARG57 | HD2 | 0.98 | 0.005 | 1.00 | 0.48 |
| ARG57 | H | 1.00 | 0.007 | 1.00 | -1803657.00 |
| ILE58 | HA | 1.00 | 0.009 | 1.00 | 0.09 |
| ILE58 | H | 1.00 | 0.006 | 1.00 | -573961.00 |
| ILE58 | HG12 | 0.51 | 0.003 | 1.00 | 0.85 |

3.57.7 Detailed Probabilities of ARG57HB2:

Overall probability: 0.538

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG57 | 0.47 | 0.88 |
| ILE58 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R57HA | 1.00 |
| R57HB3 | 1.00 |
| R57HG2 | 1.00 |
| R57HG3 | 1.00 |
| R57HD2 | 1.00 |
| R57H | 1.00 |
| R57HE | 1.00 |
| R57HB2 | 1.00 |
| I58H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG57 | HA | 1.00 | 0.156 | 0.00 | 0.00 |
| ARG57 | HB2 | 1.00 | 0.176 | 0.00 | 0.00 |
| ARG57 | HB3 | 1.00 | 0.011 | 1.00 | 3.56 |
| ARG57 | HG2 | 1.00 | 0.037 | 0.30 | 0.00 |
| ARG57 | HG3 | 1.00 | 0.072 | 0.00 | 0.00 |
| ARG57 | HD2 | 1.00 | 0.030 | 1.00 | 0.00 |
| ARG57 | H | 1.00 | 0.015 | 1.00 | -3161249.00 |
| ILE58 | H | 1.00 | 0.020 | 1.00 | -502973.00 |

3.57.8 Detailed Probabilities of ARG57HB3:

Overall probability: 0.625

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG57 | 0.71 | 0.88 |
| ILE58 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| R57HA | 1.00 |
| R57HB2 | 1.00 |
| R57HG2 | 1.00 |
| R57HG3 | 1.00 |
| R57HD2 | 1.00 |
| R57H | 1.00 |
| R57HE | 1.00 |
| R57HB3 | 1.00 |
| I58H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG57 | HA | 1.00 | 0.003 | 1.00 | 1.19 |
| ARG57 | HB2 | 1.00 | 0.329 | 0.00 | 0.00 |
| ARG57 | HB3 | 1.00 | 0.010 | 1.00 | 28.37 |
| ARG57 | HG2 | 1.00 | 0.005 | 1.00 | 1.36 |
| ARG57 | HG3 | 1.00 | 0.054 | 0.00 | 0.00 |
| ARG57 | HD2 | 1.00 | 0.016 | 1.00 | 1.32 |
| ARG57 | H | 1.00 | 0.002 | 1.00 | -1554615.00 |
| ILE58 | H | 1.00 | 0.070 | 0.00 | 0.00 |

3.57.9 Detailed Probabilities of ARG57HG2:

Overall probability: 1.000

Overall confidence: 0.800

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG57 | 1.00 | 0.78 |
| ILE58 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R57HA | 1.00 |
| R57HB2 | 1.00 |
| R57HB3 | 1.00 |
| R57HG3 | 1.00 |
| R57HD2 | 1.00 |
| R57H | 1.00 |
| R57HE | 1.00 |
| R57HH11 | 1.00 |
| R57HG2 | 1.00 |
| I58H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG57 | HA | 1.00 | 0.009 | 1.00 | 1.09 |
| ARG57 | HB2 | 1.00 | 0.009 | 1.00 | 0.98 |
| ARG57 | HB3 | 1.00 | 0.007 | 1.00 | 1.04 |
| ARG57 | HG2 | 1.00 | 0.003 | 1.00 | 27.01 |
| ARG57 | HG3 | 1.00 | 0.027 | 1.00 | 3.12 |
| ARG57 | HD2 | 1.00 | 0.002 | 1.00 | 1.77 |
| ARG57 | H | 1.00 | 0.005 | 1.00 | -1518405.00 |
| ILE58 | H | 0.97 | 0.008 | 1.00 | -1758592.00 |

3.57.10 Detailed Probabilities of ARG57HG3:

Overall probability: 0.550

Overall confidence: 0.800

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG57 | 0.49 | 0.78 |
| ILE58 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R57HA | 1.00 |
| R57HB2 | 1.00 |
| R57HB3 | 1.00 |
| R57HG2 | 1.00 |
| R57HD2 | 1.00 |
| R57H | 1.00 |
| R57HE | 1.00 |
| R57HH11 | 1.00 |
| R57HG3 | 1.00 |
| I58H | 0.96 |

NOESY contacts detailed probability

3.57 ARG(57)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG57 | HA | 1.00 | 0.110 | 0.00 | 0.00 |
| ARG57 | HB2 | 1.00 | 0.222 | 0.00 | 0.00 |
| ARG57 | HB3 | 1.00 | 0.035 | 0.50 | 0.00 |
| ARG57 | HG2 | 1.00 | 0.009 | 1.00 | 5.96 |
| ARG57 | HG3 | 1.00 | 0.053 | 0.00 | 0.00 |
| ARG57 | HD2 | 1.00 | 0.016 | 1.00 | 2.31 |
| ARG57 | H | 1.00 | 0.031 | 0.90 | 0.00 |
| ILE58 | H | 0.96 | 0.026 | 1.00 | -502973.00 |

3.57.11 Detailed Probabilities of ARG57HD2:

Overall probability: 1.000

Overall confidence: 0.667

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG57 | 1.00 | 0.67 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R57HA | 0.98 |
| R57HB2 | 1.00 |
| R57HB3 | 1.00 |
| R57HG2 | 1.00 |
| R57HG3 | 1.00 |
| R57HD3 | 1.00 |
| R57HE | 1.00 |
| R57HH11 | 1.00 |
| R57HH21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG57 | HA | 0.97 | 0.001 | 1.00 | 0.43 |
| ARG57 | HB2 | 1.00 | 0.002 | 1.00 | 0.44 |
| ARG57 | HB3 | 1.00 | 0.005 | 1.00 | 0.46 |
| ARG57 | HG2 | 1.00 | 0.001 | 1.00 | 1.23 |
| ARG57 | HG3 | 1.00 | 0.002 | 1.00 | 1.17 |
| ARG57 | HD2 | 1.00 | 0.014 | 1.00 | 52.97 |
| ARG57 | H | 0.86 | 0.008 | 1.00 | -761685.00 |

3.57.12 Detailed Probabilities of ARG57H:

Overall probability: 0.938

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE56 | 0.80 | 1.00 |
| ARG57 | 1.00 | 1.00 |
| ILE58 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F56HB2 | 1.00 |
| F56H | 1.00 |
| F56HA | 1.00 |
| F56HB3 | 1.00 |
| R57HA | 1.00 |
| R57HB2 | 1.00 |
| R57HB3 | 1.00 |
| R57HG2 | 1.00 |
| R57HG3 | 1.00 |
| R57H | 1.00 |
| I58H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE56 | HA | 1.00 | 0.031 | 0.90 | 0.00 |
| PHE56 | HB2 | 1.00 | 0.034 | 0.60 | 0.00 |
| PHE56 | HB3 | 1.00 | 0.033 | 0.70 | 0.00 |
| PHE56 | H | 1.00 | 0.016 | 1.00 | -2021385.00 |
| ARG57 | HA | 1.00 | 0.003 | 1.00 | 0.72 |
| ARG57 | HB2 | 1.00 | 0.001 | 1.00 | 0.56 |
| ARG57 | HB3 | 1.00 | 0.002 | 1.00 | 0.51 |
| ARG57 | HG2 | 1.00 | 0.000 | 1.00 | 0.61 |
| ARG57 | HG3 | 1.00 | 0.005 | 1.00 | 0.65 |
| ARG57 | H | 1.00 | 0.002 | 1.00 | -21018308.00 |
| ARG57 | HD2 | 0.87 | 0.019 | 1.00 | 0.62 |
| ILE58 | H | 1.00 | 0.002 | 1.00 | -2091708.00 |
| ILE58 | HA | 0.93 | 0.004 | 1.00 | 0.07 |

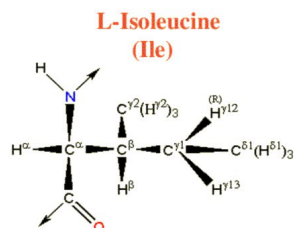


Figure 48: Image from the BMRB

Residue probability: 0.881
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|--------------|-------------|---------|--------|---------------------|--------------------|
| C | 174.794 | 175.926 | 2.710 | 0.000 | 0.000 |
| CA 3.58.1 | 61.245 | 61.717 | 4.152 | 0.945 | 1.000 |
| CB 3.58.2 | 37.027 | 38.702 | 3.945 | 0.875 | 1.000 |
| CG1 3.58.3 | 27.306 | 27.785 | 2.037 | 0.925 | 1.000 |
| CG2 3.58.4 | 16.401 | 17.574 | 1.928 | 0.750 | 1.000 |
| CD1 3.58.5 | 14.551 | 13.545 | 3.646 | 1.000 | 1.000 |
| N 3.58.6 | 122.998 | 121.467 | 6.098 | 0.941 | 1.000 |
| HA 3.58.7 | 3.859 | 4.185 | 1.403 | 0.909 | 1.000 |
| HB 3.58.8 | 2.122 | 1.776 | 0.310 | 0.875 | 1.000 |
| HG12 3.58.9 | 1.720 | 1.271 | 0.411 | 0.875 | 1.000 |
| HG13 3.58.10 | 0.911 | 1.186 | 0.426 | 0.556 | 1.000 |
| HG2 3.58.11 | 0.870 | 0.762 | 0.283 | 0.800 | 1.000 |
| HD1 3.58.12 | 0.774 | 0.668 | 0.293 | 1.000 | 1.000 |
| H 3.58.13 | 7.403 | 8.301 | 0.685 | 1.000 | 1.000 |

3.58.1 Detailed Probabilities of ILE58CA:

Overall probability: 0.945
Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|--------------|-------------|-------------|
| ARG57 | 1.00 | 1.00 |
| ILE58 | 0.91 | 1.00 |
| GLU59 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R57HA | 1.00 |
| I58HB | 1.00 |
| I58HG12 | 1.00 |
| I58HG13 | 1.00 |
| I58HG21 | 1.00 |
| I58HD11 | 0.97 |
| I58H | 1.00 |
| I58HA | 1.00 |
| E59HA | 1.00 |
| E59H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG57 | HA | 1.00 | 0.009 | 1.00 | 0.09 |
| ARG57 | H | 0.93 | 0.004 | 1.00 | 0.07 |
| ILE58 | HA | 1.00 | 0.002 | 1.00 | 6.91 |
| ILE58 | HB | 1.00 | 0.004 | 1.00 | 0.46 |
| ILE58 | HG12 | 1.00 | 0.003 | 1.00 | 0.53 |
| ILE58 | HG13 | 1.00 | 0.036 | 0.40 | 0.00 |
| ILE58 | HG21 | 1.00 | 0.005 | 1.00 | 1.77 |
| ILE58 | HD11 | 0.97 | 0.002 | 1.00 | 0.66 |
| ILE58 | H | 1.00 | 0.002 | 1.00 | 0.61 |
| GLU59 | HA | 1.00 | 0.009 | 1.00 | 0.31 |
| GLU59 | H | 1.00 | 0.001 | 1.00 | 2.81 |

3.58.2 Detailed Probabilities of ILE58CB:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE58 | 0.86 | 1.00 |
| GLU59 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I58HA | 1.00 |
| I58HG12 | 1.00 |
| I58HG13 | 1.00 |
| I58HG21 | 1.00 |
| I58HD11 | 1.00 |
| I58H | 1.00 |
| I58HB | 1.00 |
| E59H | 1.00 |

NOESY contacts detailed probability

3.58 ILE(58)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE58 | HA | 1.00 | 0.003 | 1.00 | 0.31 |
| ILE58 | HB | 1.00 | 0.000 | 1.00 | 3.58 |
| ILE58 | HG12 | 1.00 | 0.006 | 1.00 | 0.50 |
| ILE58 | HG13 | 1.00 | 0.041 | 0.00 | 0.00 |
| ILE58 | HG21 | 1.00 | 0.000 | 1.00 | 1.67 |
| ILE58 | HD11 | 1.00 | 0.007 | 1.00 | 1.96 |
| ILE58 | H | 1.00 | 0.001 | 1.00 | 1.09 |
| GLU59 | H | 1.00 | 0.003 | 1.00 | 0.11 |

3.58.3 Detailed Probabilities of ILE58CG1:

Overall probability: 0.925

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE58 | 0.91 | 1.00 |
| GLU59 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I58HA | 1.00 |
| I58HB | 1.00 |
| I58HG12 | 1.00 |
| I58HG21 | 1.00 |
| I58HD11 | 1.00 |
| I58H | 1.00 |
| I58HG13 | 1.00 |
| E59H | 0.95 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE58 | HA | 1.00 | 0.001 | 1.00 | 0.39 |
| ILE58 | HB | 1.00 | 0.001 | 1.00 | 0.31 |
| ILE58 | HG12 | 1.00 | 0.005 | 1.00 | 3.06 |
| ILE58 | HG13 | 1.00 | 0.005 | 1.00 | 2.26 |
| ILE58 | HG21 | 1.00 | 0.036 | 0.40 | 0.00 |
| ILE58 | HD11 | 1.00 | 0.007 | 1.00 | 1.30 |
| ILE58 | H | 1.00 | 0.000 | 1.00 | 0.45 |
| GLU59 | H | 0.95 | 0.008 | 1.00 | 0.10 |

3.58.4 Detailed Probabilities of ILE58CG2:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE58 | 0.71 | 1.00 |
| GLU59 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I58HA | 1.00 |
| I58HB | 1.00 |
| I58HG12 | 1.00 |
| I58HG13 | 1.00 |
| I58HG22 | 1.00 |
| I58HD11 | 0.99 |
| I58H | 1.00 |
| E59H | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE58 | HA | 1.00 | 0.001 | 1.00 | 1.12 |
| ILE58 | HB | 1.00 | 0.001 | 1.00 | 1.55 |
| ILE58 | HG12 | 1.00 | 0.196 | 0.00 | 0.00 |
| ILE58 | HG13 | 1.00 | 0.045 | 0.00 | 0.00 |
| ILE58 | HG21 | 1.00 | 0.004 | 1.00 | 40.87 |
| ILE58 | HD11 | 0.99 | 0.020 | 1.00 | 4.79 |
| ILE58 | H | 1.00 | 0.003 | 1.00 | 0.44 |
| GLU59 | H | 0.98 | 0.004 | 1.00 | 0.79 |

3.58.5 Detailed Probabilities of ILE58CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE58 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I58HA | 0.97 |
| I58HB | 1.00 |
| I58HG12 | 1.00 |
| I58HG13 | 1.00 |
| I58HG21 | 0.99 |
| I58HD12 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE58 | HA | 0.97 | 0.000 | 1.00 | 0.41 |
| ILE58 | HB | 1.00 | 0.002 | 1.00 | 1.36 |
| ILE58 | HG12 | 1.00 | 0.003 | 1.00 | 1.92 |
| ILE58 | HG13 | 1.00 | 0.030 | 1.00 | 0.00 |
| ILE58 | HG21 | 0.99 | 0.011 | 1.00 | 4.92 |
| ILE58 | HD11 | 1.00 | 0.008 | 1.00 | 40.86 |
| ILE58 | H | 0.94 | 0.002 | 1.00 | 0.67 |

3.58.6 Detailed Probabilities of ILE58N:

Overall probability: 0.941

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG57 | 0.86 | 1.00 |
| ILE58 | 1.00 | 1.00 |
| GLU59 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R57HA | 1.00 |
| R57HB2 | 1.00 |
| R57HB3 | 1.00 |
| R57HG3 | 0.96 |
| R57H | 1.00 |
| R57HG2 | 0.97 |
| I58HA | 1.00 |
| I58HB | 1.00 |
| I58HG12 | 1.00 |
| I58HG13 | 1.00 |
| I58HG21 | 1.00 |
| I58H | 1.00 |
| E59H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG57 | HA | 1.00 | 0.006 | 1.00 | -573961.00 |
| ARG57 | HB2 | 1.00 | 0.020 | 1.00 | -502973.00 |
| ARG57 | HB3 | 1.00 | 0.070 | 0.00 | 0.00 |
| ARG57 | HG2 | 0.97 | 0.008 | 1.00 | -1758592.00 |
| ARG57 | HG3 | 0.96 | 0.026 | 1.00 | -502973.00 |
| ARG57 | H | 1.00 | 0.002 | 1.00 | -2091708.00 |
| ARG57 | HD2 | 0.56 | 0.008 | 1.00 | -166840.00 |
| ILE58 | HA | 1.00 | 0.003 | 1.00 | -1000056.00 |
| ILE58 | HB | 1.00 | 0.001 | 1.00 | -2791469.00 |
| ILE58 | HG12 | 1.00 | 0.001 | 1.00 | -1758592.00 |
| ILE58 | HG13 | 1.00 | 0.026 | 1.00 | -1675496.00 |
| ILE58 | HG21 | 1.00 | 0.015 | 1.00 | -1675496.00 |
| ILE58 | H | 1.00 | 0.003 | 1.00 | -14261727.00 |
| ILE58 | HD11 | 0.94 | 0.006 | 1.00 | -1758628.00 |
| GLU59 | H | 1.00 | 0.002 | 1.00 | -323521.00 |
| GLU59 | HA | 0.93 | 0.022 | 1.00 | -400644.00 |
| GLU59 | HB2 | 0.55 | 0.023 | 1.00 | -502973.00 |

3.58.7 Detailed Probabilities of ILE58HA:

Overall probability: 0.909

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG57 | 1.00 | 1.00 |
| ILE58 | 1.00 | 1.00 |
| GLU59 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R57HA | 1.00 |
| I58HB | 1.00 |
| I58HG12 | 1.00 |
| I58HG13 | 1.00 |
| I58HG21 | 1.00 |
| I58HD11 | 0.97 |
| I58H | 1.00 |
| I58HA | 1.00 |
| E59HA | 1.00 |
| E59H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG57 | HA | 1.00 | 0.012 | 1.00 | 0.08 |
| ARG57 | H | 0.93 | 0.014 | 1.00 | -197457.00 |
| ILE58 | HA | 1.00 | 0.002 | 1.00 | 6.91 |
| ILE58 | HB | 1.00 | 0.003 | 1.00 | 0.31 |
| ILE58 | HG12 | 1.00 | 0.000 | 1.00 | 0.38 |
| ILE58 | HG13 | 1.00 | 0.001 | 1.00 | 0.39 |
| ILE58 | HG21 | 1.00 | 0.001 | 1.00 | 1.12 |
| ILE58 | HD11 | 0.97 | 0.000 | 1.00 | 0.41 |
| ILE58 | H | 1.00 | 0.003 | 1.00 | -1000056.00 |
| GLU59 | HA | 1.00 | 0.141 | 0.00 | 0.00 |
| GLU59 | H | 1.00 | 0.002 | 1.00 | -5666734.00 |

3.58.8 Detailed Probabilities of ILE58HB:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE58 | 0.86 | 1.00 |
| GLU59 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I58HA | 1.00 |
| I58HG12 | 1.00 |
| I58HG13 | 1.00 |
| I58HG21 | 1.00 |
| I58HD11 | 1.00 |
| I58H | 1.00 |
| I58HB | 1.00 |
| E59H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE58 | HA | 1.00 | 0.004 | 1.00 | 0.46 |
| ILE58 | HB | 1.00 | 0.000 | 1.00 | 3.58 |
| ILE58 | HG12 | 1.00 | 0.076 | 0.00 | 0.00 |
| ILE58 | HG13 | 1.00 | 0.001 | 1.00 | 0.31 |
| ILE58 | HG21 | 1.00 | 0.001 | 1.00 | 1.55 |
| ILE58 | HD11 | 1.00 | 0.002 | 1.00 | 1.36 |
| ILE58 | H | 1.00 | 0.001 | 1.00 | -2791469.00 |
| GLU59 | H | 1.00 | 0.008 | 1.00 | -401962.00 |

3.58.9 Detailed Probabilities of ILE58HG12:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE58 | 0.86 | 1.00 |
| GLU59 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I58HA | 1.00 |
| I58HB | 1.00 |
| I58HG13 | 1.00 |
| I58HG21 | 1.00 |
| I58HD11 | 1.00 |
| I58H | 1.00 |
| I58HG12 | 1.00 |
| E59H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE58 | HA | 1.00 | 0.003 | 1.00 | 0.53 |
| ILE58 | HB | 1.00 | 0.006 | 1.00 | 0.50 |
| ILE58 | HG12 | 1.00 | 0.010 | 1.00 | 27.01 |
| ILE58 | HG13 | 1.00 | 0.005 | 1.00 | 3.06 |
| ILE58 | HG21 | 1.00 | 0.196 | 0.00 | 0.00 |
| ILE58 | HD11 | 1.00 | 0.003 | 1.00 | 1.92 |
| ILE58 | H | 1.00 | 0.001 | 1.00 | -1758592.00 |
| GLU59 | H | 0.98 | 0.000 | 1.00 | -328925.00 |

3.58.10 Detailed Probabilities of ILE58HG13:

Overall probability: 0.556

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE58 | 0.63 | 1.00 |
| GLU59 | 0.05 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I58HA | 1.00 |
| I58HB | 1.00 |
| I58HG12 | 1.00 |
| I58HG21 | 1.00 |
| I58HD11 | 1.00 |
| I58H | 1.00 |
| I58HG13 | 1.00 |
| E59H | 0.95 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE58 | HA | 1.00 | 0.036 | 0.40 | 0.00 |
| ILE58 | HB | 1.00 | 0.041 | 0.00 | 0.00 |
| ILE58 | HG12 | 1.00 | 0.001 | 1.00 | 3.90 |
| ILE58 | HG13 | 1.00 | 0.005 | 1.00 | 2.26 |
| ILE58 | HG21 | 1.00 | 0.045 | 0.00 | 0.00 |
| ILE58 | HD11 | 1.00 | 0.030 | 1.00 | 0.00 |
| ILE58 | H | 1.00 | 0.026 | 1.00 | -1675496.00 |
| GLU59 | H | 0.95 | 0.041 | 0.05 | 0.00 |

3.58.11 Detailed Probabilities of ILE58HG21:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE58 | 0.77 | 1.00 |
| GLU59 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I58HA | 1.00 |
| I58HB | 1.00 |
| I58HG12 | 1.00 |
| I58HG13 | 1.00 |
| I58HG22 | 1.00 |
| I58HD11 | 0.99 |
| I58H | 1.00 |
| E59H | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE58 | HA | 1.00 | 0.005 | 1.00 | 1.77 |
| ILE58 | HB | 1.00 | 0.000 | 1.00 | 1.67 |
| ILE58 | HG12 | 1.00 | 0.042 | 0.00 | 0.00 |
| ILE58 | HG13 | 1.00 | 0.036 | 0.40 | 0.00 |
| ILE58 | HG21 | 1.00 | 0.004 | 1.00 | 40.87 |
| ILE58 | HD11 | 0.99 | 0.011 | 1.00 | 4.92 |
| ILE58 | H | 1.00 | 0.015 | 1.00 | -1675496.00 |
| GLU59 | H | 0.98 | 0.000 | 1.00 | -2197467.00 |

3.58.12 Detailed Probabilities of ILE58HD11:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE58 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I58HA | 0.97 |
| I58HB | 1.00 |
| I58HG12 | 1.00 |
| I58HG13 | 1.00 |
| I58HG21 | 0.99 |
| I58HD12 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE58 | HA | 0.97 | 0.002 | 1.00 | 0.66 |
| ILE58 | HB | 1.00 | 0.007 | 1.00 | 1.96 |
| ILE58 | HG12 | 1.00 | 0.002 | 1.00 | 1.47 |
| ILE58 | HG13 | 1.00 | 0.007 | 1.00 | 1.30 |
| ILE58 | HG21 | 0.99 | 0.020 | 1.00 | 4.79 |
| ILE58 | HD11 | 1.00 | 0.008 | 1.00 | 40.86 |
| ILE58 | H | 0.94 | 0.006 | 1.00 | -1758628.00 |

3.58.13 Detailed Probabilities of ILE58H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ARG57 | 1.00 | 1.00 |
| ILE58 | 1.00 | 1.00 |
| GLU59 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| R57HA | 1.00 |
| R57HB2 | 1.00 |
| R57HB3 | 1.00 |
| R57HG3 | 0.96 |
| R57H | 1.00 |
| R57HG2 | 0.97 |
| I58HA | 1.00 |
| I58HB | 1.00 |
| I58HG12 | 1.00 |
| I58HG13 | 1.00 |
| I58HG21 | 1.00 |
| I58H | 1.00 |
| E59H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ARG57 | HA | 1.00 | 0.002 | 1.00 | 0.29 |
| ARG57 | HB2 | 1.00 | 0.007 | 1.00 | 0.13 |
| ARG57 | HB3 | 1.00 | 0.002 | 1.00 | 0.09 |
| ARG57 | HG2 | 0.97 | 0.001 | 1.00 | 0.83 |
| ARG57 | HG3 | 0.96 | 0.002 | 1.00 | 0.15 |
| ARG57 | H | 1.00 | 0.002 | 1.00 | -2502456.00 |
| ILE58 | HA | 1.00 | 0.002 | 1.00 | 0.61 |
| ILE58 | HB | 1.00 | 0.001 | 1.00 | 1.09 |
| ILE58 | HG12 | 1.00 | 0.001 | 1.00 | 0.83 |
| ILE58 | HG13 | 1.00 | 0.000 | 1.00 | 0.45 |
| ILE58 | HG21 | 1.00 | 0.003 | 1.00 | 0.44 |
| ILE58 | H | 1.00 | 0.003 | 1.00 | -14261727.00 |
| ILE58 | HD11 | 0.94 | 0.002 | 1.00 | 0.67 |
| GLU59 | H | 1.00 | 0.002 | 1.00 | -393504.00 |
| GLU59 | HA | 0.93 | 0.011 | 1.00 | 0.15 |

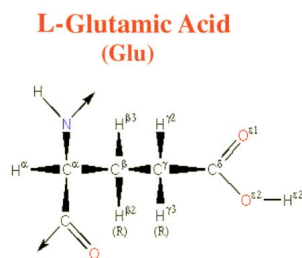
3.59 GLU(59)

Figure 49: Image from the BMRB

Residue probability: 0.681

Residue probability confidence: 0.923

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 176.355 | 176.942 | 2.547 | 0.000 | 0.000 |
| CA 3.59.1 | 58.129 | 57.442 | 3.837 | 0.727 | 1.000 |
| CB 3.59.2 | 28.735 | 30.185 | 4.018 | 0.700 | 0.875 |
| CG 3.59.3 | 36.010 | 36.085 | 1.533 | 0.843 | 0.875 |
| N 3.59.4 | 129.678 | 120.574 | 4.837 | 0.850 | 1.000 |
| HA 3.59.5 | 3.990 | 4.245 | 0.429 | 0.545 | 1.000 |
| HB2 3.59.6 | 1.941 | 2.021 | 0.233 | 0.714 | 0.875 |
| HB3 3.59.7 | 1.990 | 1.994 | 0.244 | 0.500 | 0.875 |
| HG2 3.59.8 | 2.293 | 2.258 | 0.226 | 0.429 | 0.875 |
| HG3 3.59.9 | 2.233 | 2.233 | 0.232 | 0.500 | 0.857 |
| H 3.59.10 | 8.480 | 8.332 | 0.601 | 1.000 | 1.000 |
| HE2 | NA | - | - | 0.000 | 0.000 |

3.59.1 Detailed Probabilities of GLU59CA:

Overall probability: 0.727

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE58 | 0.50 | 1.00 |
| GLU59 | 0.67 | 1.00 |
| GLY60 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| I58HA | 1.00 |
| E59HB2 | 1.00 |
| E59HB3 | 1.00 |
| E59HG2 | 1.00 |
| E59HG3 | 1.00 |
| E59H | 1.00 |
| E59HA | 1.00 |
| G60H | 1.00 |
| G60HA2 | 1.00 |
| G60HA3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE58 | HA | 1.00 | 0.141 | 0.00 | 0.00 |
| ILE58 | H | 0.93 | 0.011 | 1.00 | 0.15 |
| GLU59 | HA | 1.00 | 0.010 | 1.00 | 36.36 |
| GLU59 | HB2 | 1.00 | 0.057 | 0.00 | 0.00 |
| GLU59 | HB3 | 1.00 | 0.008 | 1.00 | 2.52 |
| GLU59 | HG2 | 1.00 | 0.063 | 0.00 | 0.00 |
| GLU59 | HG3 | 1.00 | 0.003 | 1.00 | 2.15 |
| GLU59 | H | 1.00 | 0.004 | 1.00 | 0.77 |
| GLY60 | HA2 | 1.00 | 0.003 | 1.00 | 0.23 |
| GLY60 | HA3 | 1.00 | 0.003 | 1.00 | 0.13 |
| GLY60 | H | 1.00 | 0.002 | 1.00 | 2.99 |

3.59.2 Detailed Probabilities of GLU59CB:

Overall probability: 0.700

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU59 | 0.60 | 0.86 |
| GLY60 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E59HA | 1.00 |
| E59HB3 | 1.00 |
| E59HG2 | 1.00 |
| E59HG3 | 1.00 |
| E59H | 1.00 |
| E59HE2 | 1.00 |
| E59HB2 | 1.00 |
| G60H | 1.00 |

NOESY contacts detailed probability

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU59 | HA | 1.00 | 1.768 | 0.00 | 0.00 |
| GLU59 | HB2 | 1.00 | 0.015 | 1.00 | 18.77 |
| GLU59 | HB3 | 1.00 | 0.034 | 0.60 | 0.00 |
| GLU59 | HG2 | 1.00 | 0.071 | 0.00 | 0.00 |
| GLU59 | HG3 | 1.00 | 0.011 | 1.00 | 2.87 |
| GLU59 | H | 1.00 | 0.002 | 1.00 | 1.75 |
| GLY60 | H | 1.00 | 0.001 | 1.00 | 0.40 |
| GLY60 | HA3 | 0.58 | 0.010 | 1.00 | 0.09 |

3.59.3 Detailed Probabilities of GLU59CG:

Overall probability: 0.843

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU59 | 0.82 | 0.86 |
| GLY60 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E59HA | 1.00 |
| E59HB2 | 1.00 |
| E59HB3 | 1.00 |
| E59HG3 | 1.00 |
| E59H | 1.00 |
| E59HE2 | 1.00 |
| E59HG2 | 1.00 |
| G60H | 0.96 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU59 | HA | 1.00 | 0.002 | 1.00 | 0.83 |
| GLU59 | HB2 | 1.00 | 0.018 | 1.00 | 3.06 |
| GLU59 | HB3 | 1.00 | 0.031 | 0.90 | 0.00 |
| GLU59 | HG2 | 1.00 | 0.004 | 1.00 | 51.53 |
| GLU59 | HG3 | 1.00 | 0.040 | 0.00 | 0.00 |
| GLU59 | H | 1.00 | 0.001 | 1.00 | 0.69 |
| GLY60 | H | 0.96 | 0.001 | 1.00 | 0.50 |

3.59.4 Detailed Probabilities of GLU59N:

Overall probability: 0.850

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE58 | 0.84 | 1.00 |
| GLU59 | 0.83 | 1.00 |
| GLY60 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I58HG13 | 0.95 |
| I58HG22 | 0.98 |
| I58HA | 1.00 |
| I58HG12 | 0.98 |
| I58HB | 1.00 |
| I58H | 1.00 |
| E59HA | 1.00 |
| E59HB2 | 1.00 |
| E59HB3 | 1.00 |
| E59HG2 | 1.00 |
| E59HG3 | 1.00 |
| E59H | 1.00 |
| G60H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE58 | HA | 1.00 | 0.002 | 1.00 | -5666734.00 |
| ILE58 | HB | 1.00 | 0.008 | 1.00 | -401962.00 |
| ILE58 | HG12 | 0.98 | 0.000 | 1.00 | -328925.00 |
| ILE58 | HG13 | 0.95 | 0.041 | 0.05 | 0.00 |
| ILE58 | HG21 | 0.99 | 0.000 | 1.00 | -2197467.00 |
| ILE58 | H | 1.00 | 0.002 | 1.00 | -393504.00 |
| GLU59 | HA | 1.00 | 0.001 | 1.00 | -1748941.00 |
| GLU59 | HB2 | 1.00 | 0.027 | 1.00 | -4064677.00 |
| GLU59 | HB3 | 1.00 | 0.022 | 1.00 | -4064677.00 |
| GLU59 | HG2 | 1.00 | 0.014 | 1.00 | -1050866.00 |
| GLU59 | HG3 | 1.00 | 0.046 | 0.00 | 0.00 |
| GLU59 | H | 1.00 | 0.000 | 1.00 | -19361902.00 |
| GLY60 | H | 1.00 | 0.000 | 1.00 | -447511.00 |

3.59.5 Detailed Probabilities of GLU59HA:

Overall probability: 0.545

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE58 | 1.00 | 1.00 |
| GLU59 | 0.50 | 1.00 |
| GLY60 | 0.33 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| I58HA | 1.00 |
| E59HB2 | 1.00 |
| E59HB3 | 1.00 |
| E59HG2 | 1.00 |
| E59HG3 | 1.00 |
| E59H | 1.00 |
| E59HA | 1.00 |
| G60H | 1.00 |
| G60HA2 | 1.00 |
| G60HA3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE58 | HA | 1.00 | 0.009 | 1.00 | 0.31 |
| ILE58 | H | 0.93 | 0.022 | 1.00 | -400644.00 |
| GLU59 | HA | 1.00 | 0.010 | 1.00 | 36.36 |
| GLU59 | HB2 | 1.00 | 1.768 | 0.00 | 0.00 |
| GLU59 | HB3 | 1.00 | 0.125 | 0.00 | 0.00 |
| GLU59 | HG2 | 1.00 | 0.002 | 1.00 | 0.83 |
| GLU59 | HG3 | 1.00 | 0.121 | 0.00 | 0.00 |
| GLU59 | H | 1.00 | 0.001 | 1.00 | -1748941.00 |
| GLY60 | HA2 | 1.00 | 4.280 | 0.00 | 0.00 |
| GLY60 | HA3 | 1.00 | 0.217 | 0.00 | 0.00 |
| GLY60 | H | 1.00 | 0.003 | 1.00 | -5390419.00 |

3.59.6 Detailed Probabilities of GLU59HB2:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU59 | 0.67 | 0.86 |
| GLY60 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E59HA | 1.00 |
| E59HB3 | 1.00 |
| E59HG2 | 1.00 |
| E59HG3 | 1.00 |
| E59H | 1.00 |
| E59HE2 | 1.00 |
| E59HB2 | 1.00 |
| G60H | 1.00 |

NOESY contacts detailed probability

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU59 | HA | 1.00 | 0.057 | 0.00 | 0.00 |
| GLU59 | HB2 | 1.00 | 0.015 | 1.00 | 18.77 |
| GLU59 | HB3 | 1.00 | 0.009 | 1.00 | 18.54 |
| GLU59 | HG2 | 1.00 | 0.018 | 1.00 | 3.06 |
| GLU59 | HG3 | 1.00 | 1.229 | 0.00 | 0.00 |
| GLU59 | H | 1.00 | 0.027 | 1.00 | -4064677.00 |
| GLY60 | H | 1.00 | 0.006 | 1.00 | -820474.00 |

3.59.7 Detailed Probabilities of GLU59HB3:

Overall probability: 0.500

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU59 | 0.58 | 0.86 |
| GLY60 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E59HA | 1.00 |
| E59HB2 | 1.00 |
| E59HG2 | 1.00 |
| E59HG3 | 1.00 |
| E59H | 1.00 |
| E59HE2 | 1.00 |
| E59HB3 | 1.00 |
| G60H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU59 | HA | 1.00 | 0.008 | 1.00 | 2.52 |
| GLU59 | HB2 | 1.00 | 0.034 | 0.60 | 0.00 |
| GLU59 | HB3 | 1.00 | 0.040 | 0.00 | 0.00 |
| GLU59 | HG2 | 1.00 | 0.031 | 0.90 | 0.00 |
| GLU59 | HG3 | 1.00 | 1.180 | 0.00 | 0.00 |
| GLU59 | H | 1.00 | 0.022 | 1.00 | -4064677.00 |
| GLY60 | H | 1.00 | 0.043 | 0.00 | 0.00 |

3.59.8 Detailed Probabilities of GLU59HG2:

Overall probability: 0.429

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU59 | 0.33 | 0.86 |
| GLY60 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E59HA | 1.00 |
| E59HB2 | 1.00 |
| E59HB3 | 1.00 |
| E59HG3 | 1.00 |
| E59H | 1.00 |
| E59HE2 | 1.00 |
| E59HG2 | 1.00 |
| G60H | 0.96 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU59 | HA | 1.00 | 0.063 | 0.00 | 0.00 |
| GLU59 | HB2 | 1.00 | 0.071 | 0.00 | 0.00 |
| GLU59 | HB3 | 1.00 | 0.074 | 0.00 | 0.00 |
| GLU59 | HG2 | 1.00 | 0.004 | 1.00 | 51.53 |
| GLU59 | HG3 | 1.00 | 0.877 | 0.00 | 0.00 |
| GLU59 | H | 1.00 | 0.014 | 1.00 | -1050866.00 |
| GLY60 | H | 0.96 | 0.018 | 1.00 | -630400.00 |

3.59.9 Detailed Probabilities of GLU59HG3:

Overall probability: 0.500

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU59 | 0.50 | 0.86 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E59HA | 1.00 |
| E59HB2 | 1.00 |
| E59HB3 | 1.00 |
| E59HG2 | 1.00 |
| E59H | 1.00 |
| E59HE2 | 1.00 |
| E59HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU59 | HA | 1.00 | 0.003 | 1.00 | 2.15 |
| GLU59 | HB2 | 1.00 | 0.011 | 1.00 | 2.87 |
| GLU59 | HB3 | 1.00 | 0.014 | 1.00 | 2.72 |
| GLU59 | HG2 | 1.00 | 0.040 | 0.00 | 0.00 |
| GLU59 | HG3 | 1.00 | 0.937 | 0.00 | 0.00 |
| GLU59 | H | 1.00 | 0.046 | 0.00 | 0.00 |

3.59.10 Detailed Probabilities of GLU59H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE58 | 1.00 | 1.00 |
| GLU59 | 1.00 | 1.00 |
| GLY60 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I58HG13 | 0.95 |
| I58HG22 | 0.98 |
| I58HA | 1.00 |
| I58HG12 | 0.98 |
| I58HB | 1.00 |
| I58H | 1.00 |
| E59HA | 1.00 |
| E59HB2 | 1.00 |
| E59HB3 | 1.00 |
| E59HG2 | 1.00 |
| E59HG3 | 1.00 |
| E59H | 1.00 |
| G60H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE58 | HA | 1.00 | 0.001 | 1.00 | 2.81 |
| ILE58 | HB | 1.00 | 0.003 | 1.00 | 0.11 |
| ILE58 | HG12 | 0.98 | 0.002 | 1.00 | 0.20 |
| ILE58 | HG13 | 0.95 | 0.008 | 1.00 | 0.10 |
| ILE58 | HG21 | 0.99 | 0.004 | 1.00 | 0.79 |
| ILE58 | H | 1.00 | 0.002 | 1.00 | -323521.00 |
| GLU59 | HA | 1.00 | 0.004 | 1.00 | 0.77 |
| GLU59 | HB2 | 1.00 | 0.002 | 1.00 | 1.75 |
| GLU59 | HB3 | 1.00 | 0.001 | 1.00 | 1.56 |
| GLU59 | HG2 | 1.00 | 0.001 | 1.00 | 0.69 |
| GLU59 | HG3 | 1.00 | 0.006 | 1.00 | 0.61 |
| GLU59 | H | 1.00 | 0.000 | 1.00 | -19361902.00 |
| GLY60 | H | 1.00 | 0.003 | 1.00 | -348757.00 |

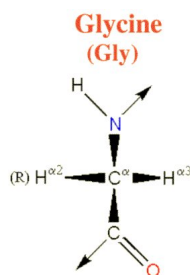
3.60 GLY(60)

Figure 50: Image from the BMRB

Residue probability: 0.563

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 174.482 | 173.872 | 2.493 | 0.000 | 0.000 |
| CA 3.60.1 | 44.262 | 45.581 | 4.381 | 0.000 | 1.000 |
| N 3.60.2 | 112.584 | 109.752 | 5.331 | 0.889 | 1.000 |
| HA2 3.60.3 | 3.528 | 3.967 | 0.380 | 0.500 | 1.000 |
| HA3 3.60.4 | 4.423 | 3.897 | 0.390 | 0.625 | 1.000 |
| H 3.60.5 | 8.682 | 8.343 | 0.939 | 0.800 | 1.000 |

3.60.1 Detailed Probabilities of GLY60CA:

Overall probability: 0.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU59 | 0.00 | 1.00 |
| GLY60 | 0.00 | 1.00 |
| VAL61 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E59HA | 1.00 |
| G60HA3 | 1.00 |
| G60H | 1.00 |
| G60HA2 | 1.00 |
| V61HA | 1.00 |
| V61H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU59 | HA | 1.00 | 4.280 | 0.00 | 0.00 |
| GLY60 | HA2 | 1.00 | 4.742 | 0.00 | 0.00 |
| GLY60 | HA3 | 1.00 | 3.847 | 0.00 | 0.00 |
| GLY60 | H | 1.00 | 0.412 | 0.00 | 0.00 |
| VAL61 | HA | 1.00 | 4.666 | 0.00 | 0.00 |
| VAL61 | H | 1.00 | 0.533 | 0.00 | 0.00 |

3.60.2 Detailed Probabilities of GLY60N:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU59 | 0.80 | 1.00 |
| GLY60 | 1.00 | 1.00 |
| VAL61 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E59HB3 | 1.00 |
| E59HB2 | 1.00 |
| E59HG2 | 0.96 |
| E59HA | 1.00 |
| E59H | 1.00 |
| G60HA2 | 1.00 |
| G60HA3 | 1.00 |
| G60H | 1.00 |
| V61H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU59 | HA | 1.00 | 0.003 | 1.00 | -5390419.00 |
| GLU59 | HB2 | 1.00 | 0.006 | 1.00 | -820474.00 |
| GLU59 | HB3 | 1.00 | 0.043 | 0.00 | 0.00 |
| GLU59 | HG2 | 0.96 | 0.018 | 1.00 | -630400.00 |
| GLU59 | H | 1.00 | 0.003 | 1.00 | -348757.00 |
| GLY60 | HA2 | 1.00 | 0.003 | 1.00 | -1836191.00 |
| GLY60 | HA3 | 1.00 | 0.004 | 1.00 | -1390435.00 |
| GLY60 | H | 1.00 | 0.001 | 1.00 | -13311573.00 |
| VAL61 | H | 1.00 | 0.003 | 1.00 | -1999610.00 |

3.60.3 Detailed Probabilities of GLY60HA2:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU59 | 1.00 | 1.00 |
| GLY60 | 0.33 | 1.00 |
| VAL61 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E59HA | 1.00 |
| G60HA3 | 1.00 |
| G60H | 1.00 |
| G60HA2 | 1.00 |
| V61HA | 1.00 |
| V61H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU59 | HA | 1.00 | 0.003 | 1.00 | 0.23 |
| GLY60 | HA2 | 1.00 | 4.742 | 0.00 | 0.00 |
| GLY60 | HA3 | 1.00 | 0.245 | 0.00 | 0.00 |
| GLY60 | H | 1.00 | 0.003 | 1.00 | -1836191.00 |
| VAL61 | HA | 1.00 | 0.387 | 0.00 | 0.00 |
| VAL61 | H | 1.00 | 0.001 | 1.00 | -853690.00 |

3.60.4 Detailed Probabilities of GLY60HA3:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU59 | 1.00 | 1.00 |
| GLY60 | 0.33 | 1.00 |
| VAL61 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E59HA | 1.00 |
| G60HA2 | 1.00 |
| G60H | 1.00 |
| G60HA3 | 1.00 |
| V61HA | 1.00 |
| V61H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU59 | HA | 1.00 | 0.003 | 1.00 | 0.13 |
| GLU59 | HB2 | 0.58 | 0.010 | 1.00 | 0.09 |
| GLU59 | HB3 | 0.74 | 0.010 | 1.00 | 0.09 |
| GLY60 | HA2 | 1.00 | 3.847 | 0.00 | 0.00 |
| GLY60 | HA3 | 1.00 | 0.323 | 0.00 | 0.00 |
| GLY60 | H | 1.00 | 0.004 | 1.00 | -1390435.00 |
| VAL61 | HA | 1.00 | 0.086 | 0.00 | 0.00 |
| VAL61 | H | 1.00 | 0.004 | 1.00 | -789874.00 |

3.60.5 Detailed Probabilities of GLY60H:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU59 | 1.00 | 1.00 |
| GLY60 | 0.33 | 1.00 |
| VAL61 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E59HB3 | 1.00 |
| E59HB2 | 1.00 |
| E59HG2 | 0.96 |
| E59HA | 1.00 |
| E59H | 1.00 |
| G60HA2 | 1.00 |
| G60HA3 | 1.00 |
| G60H | 1.00 |
| V61H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU59 | HA | 1.00 | 0.002 | 1.00 | 2.99 |
| GLU59 | HB2 | 1.00 | 0.001 | 1.00 | 0.40 |
| GLU59 | HB3 | 1.00 | 0.002 | 1.00 | 0.39 |
| GLU59 | HG2 | 0.96 | 0.001 | 1.00 | 0.50 |
| GLU59 | H | 1.00 | 0.000 | 1.00 | -447511.00 |
| GLY60 | HA2 | 1.00 | 0.412 | 0.00 | 0.00 |
| GLY60 | HA3 | 1.00 | 0.118 | 0.00 | 0.00 |
| GLY60 | H | 1.00 | 0.001 | 1.00 | -13311573.00 |
| VAL61 | H | 1.00 | 0.001 | 1.00 | -2919691.00 |
| VAL61 | HB | 0.52 | 0.020 | 1.00 | 0.32 |

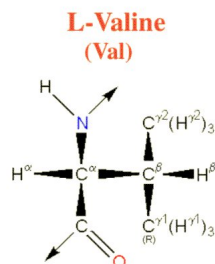
3.61 VAL(61)

Figure 51: Image from the BMRB

Residue probability: 0.800

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 174.404 | 175.682 | 2.367 | 0.000 | 0.000 |
| CA 3.61.1 | 64.836 | 62.613 | 4.828 | 0.700 | 1.000 |
| CB 3.61.2 | 31.157 | 32.918 | 4.591 | 1.000 | 1.000 |
| CG1 3.61.3 | 20.490 | 21.563 | 2.746 | 1.000 | 1.000 |
| CG2 3.61.4 | 22.302 | 21.368 | 2.801 | 0.400 | 1.000 |
| N 3.61.5 | 120.899 | 121.057 | 5.832 | 1.000 | 1.000 |
| HA 3.61.6 | 3.604 | 4.178 | 0.599 | 0.444 | 1.000 |
| HB 3.61.7 | 2.149 | 1.980 | 0.322 | 1.000 | 1.000 |
| HG1 3.61.8 | 0.243 | 0.816 | 0.264 | 0.857 | 1.000 |
| HG2 3.61.9 | 0.760 | 0.803 | 0.504 | 0.800 | 1.000 |
| H 3.61.10 | 7.737 | 8.311 | 0.669 | 0.800 | 1.000 |

3.61.1 Detailed Probabilities of VAL61CA:

Overall probability: 0.700

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLY60 | 0.00 | 1.00 |
| VAL61 | 0.80 | 1.00 |
| LYS62 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| G60HA2 | 1.00 |
| G60HA3 | 1.00 |
| V61HG11 | 1.00 |
| V61HG21 | 1.00 |
| V61H | 1.00 |
| V61HB | 1.00 |
| V61HA | 1.00 |
| K62H | 1.00 |
| K62HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLY60 | HA2 | 1.00 | 0.387 | 0.00 | 0.00 |
| GLY60 | HA3 | 1.00 | 0.086 | 0.00 | 0.00 |
| VAL61 | HA | 1.00 | 0.311 | 0.00 | 0.00 |
| VAL61 | HB | 1.00 | 0.001 | 1.00 | 0.42 |
| VAL61 | HG11 | 1.00 | 0.002 | 1.00 | 0.92 |
| VAL61 | HG21 | 1.00 | 0.000 | 1.00 | 1.39 |
| VAL61 | H | 1.00 | 0.009 | 1.00 | 0.66 |
| LYS62 | HA | 1.00 | 0.005 | 1.00 | 0.14 |
| LYS62 | H | 1.00 | 0.002 | 1.00 | 1.57 |
| LYS62 | HB2 | 0.52 | 0.009 | 1.00 | 0.19 |

3.61.2 Detailed Probabilities of VAL61CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL61 | 1.00 | 1.00 |
| LYS62 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V61HA | 1.00 |
| V61HG11 | 1.00 |
| V61HG21 | 1.00 |
| V61H | 1.00 |
| V61HB | 1.00 |
| K62H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL61 | HA | 1.00 | 0.005 | 1.00 | 0.25 |
| VAL61 | HB | 1.00 | 0.001 | 1.00 | 28.97 |
| VAL61 | HG11 | 1.00 | 0.003 | 1.00 | 1.17 |
| VAL61 | HG21 | 1.00 | 0.002 | 1.00 | 1.49 |
| VAL61 | H | 1.00 | 0.000 | 1.00 | 1.16 |
| LYS62 | H | 1.00 | 0.000 | 1.00 | 0.13 |

3.61.3 Detailed Probabilities of VAL61CG1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL61 | 1.00 | 1.00 |
| LYS62 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V61HA | 1.00 |
| V61HG12 | 1.00 |
| V61HG21 | 1.00 |
| V61H | 1.00 |
| V61HB | 1.00 |
| K62H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL61 | HA | 1.00 | 0.000 | 1.00 | 0.99 |
| VAL61 | HB | 1.00 | 0.000 | 1.00 | 1.89 |
| VAL61 | HG11 | 1.00 | 0.002 | 1.00 | 34.89 |
| VAL61 | HG21 | 1.00 | 0.003 | 1.00 | 3.20 |
| VAL61 | H | 1.00 | 0.013 | 1.00 | 1.02 |
| LYS62 | H | 0.98 | 0.002 | 1.00 | 0.62 |
| LYS62 | HA | 0.56 | 0.006 | 1.00 | 0.08 |

3.61.4 Detailed Probabilities of VAL61CG2:

Overall probability: 0.400

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL61 | 0.40 | 1.00 |
| LYS62 | NaN | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V61HA | 1.00 |
| V61HG11 | 1.00 |
| V61HG22 | 1.00 |
| V61H | 1.00 |
| V61HB | 1.00 |
| K62H | 0.95 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL61 | HA | 1.00 | 0.259 | 0.00 | 0.00 |
| VAL61 | HB | 1.00 | 0.011 | 1.00 | 2.87 |
| VAL61 | HG11 | 1.00 | 0.345 | 0.00 | 0.00 |
| VAL61 | HG21 | 1.00 | 0.102 | 0.00 | 0.00 |
| VAL61 | H | 1.00 | 0.002 | 1.00 | 1.48 |

3.61.5 Detailed Probabilities of VAL61N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLY60 | 1.00 | 1.00 |
| VAL61 | 1.00 | 1.00 |
| LYS62 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| G60H | 1.00 |
| G60HA2 | 1.00 |
| G60HA3 | 1.00 |
| V61HA | 1.00 |
| V61HG11 | 1.00 |
| V61HG21 | 1.00 |
| V61HB | 1.00 |
| V61H | 1.00 |
| K62H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLY60 | HA2 | 1.00 | 0.001 | 1.00 | -853690.00 |
| GLY60 | HA3 | 1.00 | 0.004 | 1.00 | -789874.00 |
| GLY60 | H | 1.00 | 0.001 | 1.00 | -2919691.00 |
| VAL61 | HA | 1.00 | 0.005 | 1.00 | -1225302.00 |
| VAL61 | HB | 1.00 | 0.002 | 1.00 | -4517898.00 |
| VAL61 | HG11 | 1.00 | 0.005 | 1.00 | -1215219.00 |
| VAL61 | HG21 | 1.00 | 0.001 | 1.00 | -3941008.00 |
| VAL61 | H | 1.00 | 0.001 | 1.00 | -21402160.00 |
| LYS62 | H | 1.00 | 0.005 | 1.00 | -326786.00 |
| LYS62 | HA | 0.91 | 0.002 | 1.00 | -101131.00 |

3.61.6 Detailed Probabilities of VAL61HA:

Overall probability: 0.444

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLY60 | 0.00 | 1.00 |
| VAL61 | 0.60 | 1.00 |
| LYS62 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| G60HA2 | 1.00 |
| G60HA3 | 1.00 |
| V61HG11 | 1.00 |
| V61HG21 | 1.00 |
| V61H | 1.00 |
| V61HB | 1.00 |
| V61HA | 1.00 |
| K62H | 1.00 |
| K62HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLY60 | HA2 | 1.00 | 4.666 | 0.00 | 0.00 |
| GLY60 | HA3 | 1.00 | 0.169 | 0.00 | 0.00 |
| VAL61 | HA | 1.00 | 0.311 | 0.00 | 0.00 |
| VAL61 | HB | 1.00 | 0.005 | 1.00 | 0.25 |
| VAL61 | HG11 | 1.00 | 0.000 | 1.00 | 0.99 |
| VAL61 | HG21 | 1.00 | 0.259 | 0.00 | 0.00 |
| VAL61 | H | 1.00 | 0.005 | 1.00 | -1225302.00 |
| LYS62 | HA | 1.00 | 0.187 | 0.00 | 0.00 |
| LYS62 | H | 1.00 | 0.002 | 1.00 | -2993094.00 |

3.61.7 Detailed Probabilities of VAL61HB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL61 | 1.00 | 1.00 |
| LYS62 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V61HA | 1.00 |
| V61HG11 | 1.00 |
| V61HG21 | 1.00 |
| V61H | 1.00 |
| V61HB | 1.00 |
| K62H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL61 | HA | 1.00 | 0.001 | 1.00 | 0.42 |
| VAL61 | HB | 1.00 | 0.001 | 1.00 | 28.97 |
| VAL61 | HG11 | 1.00 | 0.000 | 1.00 | 1.89 |
| VAL61 | HG21 | 1.00 | 0.011 | 1.00 | 2.87 |
| VAL61 | H | 1.00 | 0.002 | 1.00 | -4517898.00 |
| LYS62 | H | 1.00 | 0.015 | 1.00 | -237358.00 |
| LYS62 | HA | 0.81 | 0.026 | 1.00 | 0.18 |

3.61.8 Detailed Probabilities of VAL61HG11:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL61 | 0.80 | 1.00 |
| LYS62 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V61HA | 1.00 |
| V61HG12 | 1.00 |
| V61HG21 | 1.00 |
| V61H | 1.00 |
| V61HB | 1.00 |
| K62H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL61 | HA | 1.00 | 0.002 | 1.00 | 0.92 |
| VAL61 | HB | 1.00 | 0.003 | 1.00 | 1.17 |
| VAL61 | HG11 | 1.00 | 0.002 | 1.00 | 34.89 |
| VAL61 | HG21 | 1.00 | 0.345 | 0.00 | 0.00 |
| VAL61 | H | 1.00 | 0.005 | 1.00 | -1215219.00 |
| LYS62 | H | 0.98 | 0.002 | 1.00 | -1035587.00 |
| LYS62 | HA | 0.56 | 0.018 | 1.00 | 0.18 |

3.61.9 Detailed Probabilities of VAL61HG21:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL61 | 0.80 | 1.00 |
| LYS62 | NaN | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V61HA | 1.00 |
| V61HG11 | 1.00 |
| V61HG22 | 1.00 |
| V61H | 1.00 |
| V61HB | 1.00 |
| K62H | 0.95 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL61 | HA | 1.00 | 0.000 | 1.00 | 1.39 |
| VAL61 | HB | 1.00 | 0.002 | 1.00 | 1.49 |
| VAL61 | HG11 | 1.00 | 0.003 | 1.00 | 3.20 |
| VAL61 | HG21 | 1.00 | 0.102 | 0.00 | 0.00 |
| VAL61 | H | 1.00 | 0.001 | 1.00 | -3941008.00 |

3.61.10 Detailed Probabilities of VAL61H:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLY60 | 0.33 | 1.00 |
| VAL61 | 1.00 | 1.00 |
| LYS62 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| G60H | 1.00 |
| G60HA2 | 1.00 |
| G60HA3 | 1.00 |
| V61HA | 1.00 |
| V61HG11 | 1.00 |
| V61HG21 | 1.00 |
| V61HB | 1.00 |
| V61H | 1.00 |
| K62H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLY60 | HA2 | 1.00 | 0.533 | 0.00 | 0.00 |
| GLY60 | HA3 | 1.00 | 0.354 | 0.00 | 0.00 |
| GLY60 | H | 1.00 | 0.003 | 1.00 | -1999610.00 |
| VAL61 | HA | 1.00 | 0.009 | 1.00 | 0.66 |
| VAL61 | HB | 1.00 | 0.000 | 1.00 | 1.16 |
| VAL61 | HG11 | 1.00 | 0.013 | 1.00 | 1.02 |
| VAL61 | HG21 | 1.00 | 0.002 | 1.00 | 1.48 |
| VAL61 | H | 1.00 | 0.001 | 1.00 | -21402160.00 |
| LYS62 | H | 1.00 | 0.023 | 1.00 | -1891826.00 |
| LYS62 | HA | 0.91 | 0.026 | 1.00 | 0.40 |

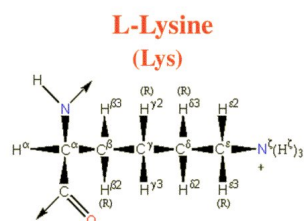


Figure 52: Image from the BMRB

Residue probability: 0.591
 Residue probability confidence: 0.945

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 174.846 | 176.660 | 3.133 | 0.000 | 0.000 |
| CA 3.62.1 | 56.624 | 57.014 | 3.028 | 0.793 | 1.000 |
| CB 3.62.2 | 35.500 | 32.981 | 3.186 | 0.273 | 1.000 |
| CG 3.62.3 | 24.553 | 24.941 | 1.956 | 0.845 | 0.917 |
| CD 3.62.4 | 29.505 | 29.020 | 2.193 | 0.770 | 0.900 |
| CE 3.62.5 | 41.780 | 41.893 | 1.492 | 0.114 | 0.889 |
| N 3.62.6 | 130.818 | 120.954 | 4.210 | 1.000 | 1.000 |
| NZ | NA | – | – | 0.000 | 0.000 |
| HA 3.62.7 | 4.514 | 4.262 | 0.489 | 0.867 | 1.000 |
| HB2 3.62.8 | 1.426 | 1.774 | 0.365 | 0.669 | 1.000 |
| HB3 3.62.9 | 1.345 | 1.742 | 0.385 | 0.184 | 1.000 |
| HG2 3.62.10 | 1.556 | 1.358 | 0.344 | 0.455 | 0.917 |
| HG3 3.62.11 | 1.416 | 1.343 | 0.357 | 0.636 | 0.917 |
| HD2 3.62.12 | 1.603 | 1.614 | 0.957 | 0.156 | 0.900 |
| HD3 3.62.13 | 1.740 | 1.595 | 0.387 | 0.570 | 0.900 |
| HE2 3.62.14 | 3.058 | 2.907 | 0.230 | 0.627 | 0.889 |
| HE3 3.62.15 | 3.060 | 2.901 | 0.241 | 0.626 | 0.889 |
| H 3.62.16 | 9.311 | 8.185 | 0.605 | 0.867 | 1.000 |
| HZ | NA | – | – | 0.000 | 0.000 |

3.62.1 Detailed Probabilities of LYS62CA:

Overall probability: 0.793
 Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL61 | 0.75 | 1.00 |
| LYS62 | 0.89 | 1.00 |
| SER63 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| V61HA | 1.00 |
| K62HB2 | 1.00 |
| K62HB3 | 1.00 |
| K62HG2 | 1.00 |
| K62HG3 | 1.00 |
| K62HD2 | 0.98 |
| K62HD3 | 0.98 |
| K62H | 1.00 |
| K62HA | 1.00 |
| S63HA | 1.00 |
| S63H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL61 | HA | 1.00 | 0.187 | 0.00 | 0.00 |
| VAL61 | HB | 0.81 | 0.026 | 1.00 | 0.18 |
| VAL61 | HG11 | 0.59 | 0.018 | 1.00 | 0.18 |
| VAL61 | H | 0.91 | 0.026 | 1.00 | 0.40 |
| LYS62 | HA | 1.00 | 0.011 | 1.00 | 111.89 |
| LYS62 | HB2 | 1.00 | 0.000 | 1.00 | 1.32 |
| LYS62 | HB3 | 1.00 | 0.000 | 1.00 | 1.09 |
| LYS62 | HG2 | 1.00 | 0.008 | 1.00 | 0.95 |
| LYS62 | HG3 | 1.00 | 0.010 | 1.00 | 1.32 |
| LYS62 | HD2 | 0.98 | 0.039 | 0.10 | 0.00 |
| LYS62 | HD3 | 0.98 | 0.006 | 1.00 | 0.25 |
| LYS62 | H | 1.00 | 0.003 | 1.00 | 0.57 |
| SER63 | HA | 1.00 | 0.057 | 0.00 | 0.00 |
| SER63 | H | 1.00 | 0.002 | 1.00 | 0.40 |

3.62.2 Detailed Probabilities of LYS62CB:

Overall probability: 0.273

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS62 | 0.20 | 1.00 |
| SER63 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K62HA | 1.00 |
| K62HB2 | 1.00 |
| K62HG2 | 1.00 |
| K62HG3 | 1.00 |
| K62HD2 | 1.00 |
| K62HD3 | 1.00 |
| K62HE2 | 0.99 |
| K62HE3 | 0.99 |
| K62H | 1.00 |
| K62HB3 | 1.00 |
| S63H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS62 | HA | 1.00 | 1.459 | 0.00 | 0.00 |
| LYS62 | HB2 | 1.00 | 0.478 | 0.00 | 0.00 |
| LYS62 | HB3 | 1.00 | 0.559 | 0.00 | 0.00 |
| LYS62 | HG2 | 1.00 | 0.348 | 0.00 | 0.00 |
| LYS62 | HG3 | 1.00 | 0.488 | 0.00 | 0.00 |
| LYS62 | HD2 | 1.00 | 0.301 | 0.00 | 0.00 |
| LYS62 | HD3 | 1.00 | 0.164 | 0.00 | 0.00 |
| LYS62 | HE2 | 0.99 | 0.003 | 1.00 | 0.11 |
| LYS62 | HE3 | 0.99 | 0.005 | 1.00 | 0.11 |
| LYS62 | H | 1.00 | 1.038 | 0.00 | 0.00 |
| SER63 | H | 1.00 | 0.002 | 1.00 | 0.15 |

3.62.3 Detailed Probabilities of LYS62CG:

Overall probability: 0.845

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS62 | 0.83 | 0.91 |
| SER63 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K62HA | 1.00 |
| K62HB2 | 1.00 |
| K62HB3 | 1.00 |
| K62HG3 | 1.00 |
| K62HD2 | 1.00 |
| K62HD3 | 1.00 |
| K62HE2 | 1.00 |
| K62HE3 | 1.00 |
| K62H | 1.00 |
| K62HZ2 | 1.00 |
| K62HG2 | 1.00 |
| S63H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS62 | HA | 1.00 | 0.002 | 1.00 | 0.49 |
| LYS62 | HB2 | 1.00 | 0.007 | 1.00 | 3.08 |
| LYS62 | HB3 | 1.00 | 0.074 | 0.00 | 0.00 |
| LYS62 | HG2 | 1.00 | 0.010 | 1.00 | 3.88 |
| LYS62 | HG3 | 1.00 | 0.003 | 1.00 | 3.08 |
| LYS62 | HD2 | 1.00 | 0.037 | 0.30 | 0.00 |
| LYS62 | HD3 | 1.00 | 0.009 | 1.00 | 1.01 |
| LYS62 | HE2 | 1.00 | 0.001 | 1.00 | 0.65 |
| LYS62 | HE3 | 1.00 | 0.003 | 1.00 | 0.65 |
| LYS62 | H | 1.00 | 0.003 | 1.00 | 0.14 |
| SER63 | H | 0.97 | 0.010 | 1.00 | 0.10 |

3.62.4 Detailed Probabilities of LYS62CD:

Overall probability: 0.770

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS62 | 0.77 | 0.90 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K62HA | 0.98 |
| K62HB2 | 1.00 |
| K62HB3 | 1.00 |
| K62HG2 | 1.00 |
| K62HG3 | 1.00 |
| K62HD2 | 1.00 |
| K62HE2 | 1.00 |
| K62HE3 | 1.00 |
| K62HZ2 | 1.00 |
| K62HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS62 | HA | 0.98 | 0.006 | 1.00 | 0.24 |
| LYS62 | HB2 | 1.00 | 0.006 | 1.00 | 1.13 |
| LYS62 | HB3 | 1.00 | 0.075 | 0.00 | 0.00 |
| LYS62 | HG2 | 1.00 | 0.041 | 0.00 | 0.00 |
| LYS62 | HG3 | 1.00 | 0.004 | 1.00 | 1.13 |
| LYS62 | HD2 | 1.00 | 0.006 | 1.00 | 4.42 |
| LYS62 | HD3 | 1.00 | 0.033 | 0.70 | 0.00 |
| LYS62 | HE2 | 1.00 | 0.002 | 1.00 | 1.25 |
| LYS62 | HE3 | 1.00 | 0.004 | 1.00 | 1.25 |
| LYS62 | H | 0.87 | 0.001 | 1.00 | 0.08 |

3.62.5 Detailed Probabilities of LYS62CE:

Overall probability: 0.114

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS62 | 0.11 | 0.89 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K62HB2 | 0.98 |
| K62HB3 | 0.99 |
| K62HG2 | 1.00 |
| K62HG3 | 1.00 |
| K62HD2 | 1.00 |
| K62HD3 | 1.00 |
| K62HE3 | 1.00 |
| K62HZ2 | 1.00 |
| K62HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS62 | HB2 | 0.98 | 0.459 | 0.02 | 0.00 |
| LYS62 | HB3 | 0.99 | 0.532 | 0.01 | 0.00 |
| LYS62 | HG2 | 1.00 | 0.329 | 0.00 | 0.00 |
| LYS62 | HG3 | 1.00 | 0.469 | 0.00 | 0.00 |
| LYS62 | HD2 | 1.00 | 0.282 | 0.00 | 0.00 |
| LYS62 | HD3 | 1.00 | 0.145 | 0.00 | 0.00 |
| LYS62 | HE2 | 1.00 | 0.151 | 0.00 | 0.00 |
| LYS62 | HE3 | 1.00 | 0.153 | 0.00 | 0.00 |
| LYS62 | HA | 0.77 | 0.002 | 1.00 | 0.17 |

3.62.6 Detailed Probabilities of LYS62N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL61 | 1.00 | 1.00 |
| LYS62 | 1.00 | 1.00 |
| SER63 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V61HA | 1.00 |
| V61HG21 | 0.95 |
| V61H | 1.00 |
| V61HG11 | 0.98 |
| V61HB | 1.00 |
| K62HA | 1.00 |
| K62HB2 | 1.00 |
| K62HB3 | 1.00 |
| K62HG2 | 1.00 |
| K62HG3 | 1.00 |
| K62H | 1.00 |
| S63H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL61 | HA | 1.00 | 0.002 | 1.00 | -2993094.00 |
| VAL61 | HB | 1.00 | 0.015 | 1.00 | -237358.00 |
| VAL61 | HG11 | 0.98 | 0.002 | 1.00 | -1035587.00 |
| VAL61 | HG21 | 0.95 | 0.000 | 1.00 | -698754.00 |
| VAL61 | H | 1.00 | 0.023 | 1.00 | -1891826.00 |
| LYS62 | HA | 1.00 | 0.003 | 1.00 | -645615.00 |
| LYS62 | HB2 | 1.00 | 0.001 | 1.00 | -1310803.00 |
| LYS62 | HB3 | 1.00 | 0.021 | 1.00 | -880713.00 |
| LYS62 | HG2 | 1.00 | 0.008 | 1.00 | -470350.00 |
| LYS62 | HG3 | 1.00 | 0.009 | 1.00 | -1310803.00 |
| LYS62 | H | 1.00 | 0.002 | 1.00 | -6220846.00 |
| LYS62 | HD3 | 0.87 | 0.009 | 1.00 | -138508.00 |
| SER63 | H | 1.00 | 0.001 | 1.00 | -1891826.00 |
| SER63 | HA | 0.87 | 0.010 | 1.00 | -113727.00 |

3.62.7 Detailed Probabilities of LYS62HA:

Overall probability: 0.867

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL61 | 1.00 | 1.00 |
| LYS62 | 0.80 | 1.00 |
| SER63 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| V61HA | 1.00 |
| K62HB2 | 1.00 |
| K62HB3 | 1.00 |
| K62HG2 | 1.00 |
| K62HG3 | 1.00 |
| K62HD2 | 0.98 |
| K62HD3 | 0.98 |
| K62H | 1.00 |
| K62HA | 1.00 |
| S63HA | 1.00 |
| S63H | 1.00 |

NOESY contacts detailed probability

3.62 LYS(62)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL61 | HA | 1.00 | 0.005 | 1.00 | 0.14 |
| VAL61 | HG11 | 0.59 | 0.006 | 1.00 | 0.08 |
| VAL61 | H | 0.91 | 0.002 | 1.00 | -101131.00 |
| LYS62 | HA | 1.00 | 0.011 | 1.00 | 111.89 |
| LYS62 | HB2 | 1.00 | 0.793 | 0.00 | 0.00 |
| LYS62 | HB3 | 1.00 | 1.459 | 0.00 | 0.00 |
| LYS62 | HG2 | 1.00 | 0.002 | 1.00 | 0.49 |
| LYS62 | HG3 | 1.00 | 0.001 | 1.00 | 0.42 |
| LYS62 | HD2 | 0.98 | 0.005 | 1.00 | 0.23 |
| LYS62 | HD3 | 0.98 | 0.006 | 1.00 | 0.24 |
| LYS62 | H | 1.00 | 0.003 | 1.00 | -645615.00 |
| LYS62 | HE2 | 0.77 | 0.002 | 1.00 | 0.17 |
| LYS62 | HE3 | 0.76 | 0.002 | 1.00 | 0.17 |
| SER63 | HA | 1.00 | 0.024 | 1.00 | 1.11 |
| SER63 | H | 1.00 | 0.004 | 1.00 | -633644.00 |

3.62.8 Detailed Probabilities of LYS62HB2:

Overall probability: 0.669

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS62 | 0.60 | 1.00 |
| SER63 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K62HA | 1.00 |
| K62HB3 | 1.00 |
| K62HG2 | 1.00 |
| K62HG3 | 1.00 |
| K62HD2 | 1.00 |
| K62HD3 | 1.00 |
| K62HE2 | 0.98 |
| K62HE3 | 0.99 |
| K62H | 1.00 |
| K62HB2 | 1.00 |
| S63H | 1.00 |

NOESY contacts detailed probability

3.62 LYS(62)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS62 | HA | 1.00 | 0.000 | 1.00 | 1.32 |
| LYS62 | HB2 | 1.00 | 0.221 | 0.00 | 0.00 |
| LYS62 | HB3 | 1.00 | 0.478 | 0.00 | 0.00 |
| LYS62 | HG2 | 1.00 | 0.007 | 1.00 | 3.08 |
| LYS62 | HG3 | 1.00 | 0.011 | 1.00 | 5.33 |
| LYS62 | HD2 | 1.00 | 0.006 | 1.00 | 1.58 |
| LYS62 | HD3 | 1.00 | 0.006 | 1.00 | 1.13 |
| LYS62 | HE2 | 0.98 | 0.459 | 0.02 | 0.00 |
| LYS62 | HE3 | 0.99 | 0.459 | 0.01 | 0.00 |
| LYS62 | H | 1.00 | 0.001 | 1.00 | -1310803.00 |
| SER63 | H | 1.00 | 0.001 | 1.00 | -1444562.00 |
| SER63 | HA | 0.67 | 0.015 | 1.00 | 0.22 |

3.62.9 Detailed Probabilities of LYS62HB3:

Overall probability: 0.184

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS62 | 0.20 | 1.00 |
| SER63 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K62HA | 1.00 |
| K62HB2 | 1.00 |
| K62HG2 | 1.00 |
| K62HG3 | 1.00 |
| K62HD2 | 1.00 |
| K62HD3 | 1.00 |
| K62HE2 | 0.99 |
| K62HE3 | 0.99 |
| K62H | 1.00 |
| K62HB3 | 1.00 |
| S63H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS62 | HA | 1.00 | 0.000 | 1.00 | 1.09 |
| LYS62 | HB2 | 1.00 | 0.140 | 0.00 | 0.00 |
| LYS62 | HB3 | 1.00 | 0.559 | 0.00 | 0.00 |
| LYS62 | HG2 | 1.00 | 0.074 | 0.00 | 0.00 |
| LYS62 | HG3 | 1.00 | 0.070 | 0.00 | 0.00 |
| LYS62 | HD2 | 1.00 | 0.075 | 0.00 | 0.00 |
| LYS62 | HD3 | 1.00 | 0.075 | 0.00 | 0.00 |
| LYS62 | HE2 | 0.99 | 0.532 | 0.01 | 0.00 |
| LYS62 | HE3 | 0.99 | 0.532 | 0.01 | 0.00 |
| LYS62 | H | 1.00 | 0.021 | 1.00 | -880713.00 |
| SER63 | H | 1.00 | 0.080 | 0.00 | 0.00 |

3.62.10 Detailed Probabilities of LYS62HG2:

Overall probability: 0.455

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS62 | 0.40 | 0.91 |
| SER63 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K62HA | 1.00 |
| K62HB2 | 1.00 |
| K62HB3 | 1.00 |
| K62HG3 | 1.00 |
| K62HD2 | 1.00 |
| K62HD3 | 1.00 |
| K62HE2 | 1.00 |
| K62HE3 | 1.00 |
| K62H | 1.00 |
| K62HZ2 | 1.00 |
| K62HG2 | 1.00 |
| S63H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS62 | HA | 1.00 | 0.008 | 1.00 | 0.95 |
| LYS62 | HB2 | 1.00 | 0.351 | 0.00 | 0.00 |
| LYS62 | HB3 | 1.00 | 0.348 | 0.00 | 0.00 |
| LYS62 | HG2 | 1.00 | 0.010 | 1.00 | 3.88 |
| LYS62 | HG3 | 1.00 | 0.005 | 1.00 | 3.07 |
| LYS62 | HD2 | 1.00 | 0.136 | 0.00 | 0.00 |
| LYS62 | HD3 | 1.00 | 0.041 | 0.00 | 0.00 |
| LYS62 | HE2 | 1.00 | 0.329 | 0.00 | 0.00 |
| LYS62 | HE3 | 1.00 | 0.329 | 0.00 | 0.00 |
| LYS62 | H | 1.00 | 0.008 | 1.00 | -470350.00 |
| SER63 | H | 0.97 | 0.001 | 1.00 | -406648.00 |

3.62.11 Detailed Probabilities of LYS62HG3:

Overall probability: 0.636

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS62 | 0.60 | 0.91 |
| SER63 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K62HA | 1.00 |
| K62HB2 | 1.00 |
| K62HB3 | 1.00 |
| K62HG2 | 1.00 |
| K62HD2 | 1.00 |
| K62HD3 | 1.00 |
| K62HE2 | 1.00 |
| K62HE3 | 1.00 |
| K62H | 1.00 |
| K62HZ2 | 1.00 |
| K62HG3 | 1.00 |
| S63H | 0.96 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS62 | HA | 1.00 | 0.010 | 1.00 | 1.32 |
| LYS62 | HB2 | 1.00 | 0.211 | 0.00 | 0.00 |
| LYS62 | HB3 | 1.00 | 0.488 | 0.00 | 0.00 |
| LYS62 | HG2 | 1.00 | 0.003 | 1.00 | 3.08 |
| LYS62 | HG3 | 1.00 | 0.001 | 1.00 | 5.33 |
| LYS62 | HD2 | 1.00 | 0.004 | 1.00 | 1.58 |
| LYS62 | HD3 | 1.00 | 0.004 | 1.00 | 1.13 |
| LYS62 | HE2 | 1.00 | 0.469 | 0.00 | 0.00 |
| LYS62 | HE3 | 1.00 | 0.469 | 0.00 | 0.00 |
| LYS62 | H | 1.00 | 0.009 | 1.00 | -1310803.00 |
| SER63 | H | 0.96 | 0.009 | 1.00 | -1444562.00 |

3.62.12 Detailed Probabilities of LYS62HD2:

Overall probability: 0.156

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS62 | 0.16 | 0.90 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K62HA | 0.98 |
| K62HB2 | 1.00 |
| K62HB3 | 1.00 |
| K62HG2 | 1.00 |
| K62HG3 | 1.00 |
| K62HD3 | 1.00 |
| K62HE2 | 1.00 |
| K62HE3 | 1.00 |
| K62HZ2 | 1.00 |
| K62HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS62 | HA | 0.98 | 0.039 | 0.10 | 0.00 |
| LYS62 | HB2 | 1.00 | 0.398 | 0.00 | 0.00 |
| LYS62 | HB3 | 1.00 | 0.301 | 0.00 | 0.00 |
| LYS62 | HG2 | 1.00 | 0.037 | 0.30 | 0.00 |
| LYS62 | HG3 | 1.00 | 0.042 | 0.00 | 0.00 |
| LYS62 | HD2 | 1.00 | 0.128 | 0.00 | 0.00 |
| LYS62 | HD3 | 1.00 | 0.006 | 1.00 | 4.42 |
| LYS62 | HE2 | 1.00 | 0.282 | 0.00 | 0.00 |
| LYS62 | HE3 | 1.00 | 0.282 | 0.00 | 0.00 |

3.62.13 Detailed Probabilities of LYS62HD3:

Overall probability: 0.570

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS62 | 0.57 | 0.90 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K62HA | 0.98 |
| K62HB2 | 1.00 |
| K62HB3 | 1.00 |
| K62HG2 | 1.00 |
| K62HG3 | 1.00 |
| K62HD2 | 1.00 |
| K62HE2 | 1.00 |
| K62HE3 | 1.00 |
| K62HZ2 | 1.00 |
| K62HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS62 | HA | 0.98 | 0.006 | 1.00 | 0.25 |
| LYS62 | HB2 | 1.00 | 0.535 | 0.00 | 0.00 |
| LYS62 | HB3 | 1.00 | 0.164 | 0.00 | 0.00 |
| LYS62 | HG2 | 1.00 | 0.009 | 1.00 | 1.01 |
| LYS62 | HG3 | 1.00 | 0.014 | 1.00 | 0.62 |
| LYS62 | HD2 | 1.00 | 0.009 | 1.00 | 3.56 |
| LYS62 | HD3 | 1.00 | 0.033 | 0.70 | 0.00 |
| LYS62 | HE2 | 1.00 | 0.145 | 0.00 | 0.00 |
| LYS62 | HE3 | 1.00 | 0.145 | 0.00 | 0.00 |
| LYS62 | H | 0.87 | 0.009 | 1.00 | -138508.00 |

3.62.14 Detailed Probabilities of LYS62HE2:

Overall probability: 0.627

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS62 | 0.63 | 0.89 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K62HB2 | 0.98 |
| K62HB3 | 0.99 |
| K62HG2 | 1.00 |
| K62HG3 | 1.00 |
| K62HD2 | 1.00 |
| K62HD3 | 1.00 |
| K62HE3 | 1.00 |
| K62HZ2 | 1.00 |
| K62HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS62 | HB2 | 0.98 | 1.853 | 0.02 | 0.00 |
| LYS62 | HB3 | 0.99 | 0.003 | 1.00 | 0.11 |
| LYS62 | HG2 | 1.00 | 0.001 | 1.00 | 0.65 |
| LYS62 | HG3 | 1.00 | 0.001 | 1.00 | 0.68 |
| LYS62 | HD2 | 1.00 | 0.000 | 1.00 | 1.14 |
| LYS62 | HD3 | 1.00 | 0.002 | 1.00 | 1.25 |
| LYS62 | HE2 | 1.00 | 0.151 | 0.00 | 0.00 |
| LYS62 | HE3 | 1.00 | 0.151 | 0.00 | 0.00 |

3.62.15 Detailed Probabilities of LYS62HE3:

Overall probability: 0.626

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS62 | 0.63 | 0.89 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K62HB2 | 0.99 |
| K62HB3 | 0.99 |
| K62HG2 | 1.00 |
| K62HG3 | 1.00 |
| K62HD2 | 1.00 |
| K62HD3 | 1.00 |
| K62HE2 | 1.00 |
| K62HZ2 | 1.00 |
| K62HE3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS62 | HB2 | 0.99 | 1.855 | 0.01 | 0.00 |
| LYS62 | HB3 | 0.99 | 0.005 | 1.00 | 0.11 |
| LYS62 | HG2 | 1.00 | 0.003 | 1.00 | 0.65 |
| LYS62 | HG3 | 1.00 | 0.003 | 1.00 | 0.68 |
| LYS62 | HD2 | 1.00 | 0.002 | 1.00 | 1.14 |
| LYS62 | HD3 | 1.00 | 0.004 | 1.00 | 1.25 |
| LYS62 | HE2 | 1.00 | 0.153 | 0.00 | 0.00 |
| LYS62 | HE3 | 1.00 | 0.153 | 0.00 | 0.00 |

3.62.16 Detailed Probabilities of LYS62H:

Overall probability: 0.867

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL61 | 1.00 | 1.00 |
| LYS62 | 0.75 | 1.00 |
| SER63 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V61HA | 1.00 |
| V61HG21 | 0.95 |
| V61H | 1.00 |
| V61HG11 | 0.98 |
| V61HB | 1.00 |
| K62HA | 1.00 |
| K62HB2 | 1.00 |
| K62HB3 | 1.00 |
| K62HG2 | 1.00 |
| K62HG3 | 1.00 |
| K62H | 1.00 |
| S63H | 1.00 |

NOESY contacts detailed probability

3.62 LYS(62)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL61 | HA | 1.00 | 0.002 | 1.00 | 1.57 |
| VAL61 | HB | 1.00 | 0.000 | 1.00 | 0.13 |
| VAL61 | HG11 | 0.98 | 0.002 | 1.00 | 0.62 |
| VAL61 | HG21 | 0.95 | 0.003 | 1.00 | 0.36 |
| VAL61 | H | 1.00 | 0.005 | 1.00 | -326786.00 |
| LYS62 | HA | 1.00 | 0.003 | 1.00 | 0.57 |
| LYS62 | HB2 | 1.00 | 4.004 | 0.00 | 0.00 |
| LYS62 | HB3 | 1.00 | 1.038 | 0.00 | 0.00 |
| LYS62 | HG2 | 1.00 | 0.003 | 1.00 | 0.14 |
| LYS62 | HG3 | 1.00 | 0.006 | 1.00 | 0.19 |
| LYS62 | H | 1.00 | 0.002 | 1.00 | -6220846.00 |
| LYS62 | HD2 | 0.88 | 0.004 | 1.00 | 0.09 |
| LYS62 | HD3 | 0.87 | 0.001 | 1.00 | 0.08 |
| SER63 | H | 1.00 | 0.001 | 1.00 | -2741988.00 |
| SER63 | HA | 0.87 | 0.005 | 1.00 | 0.09 |

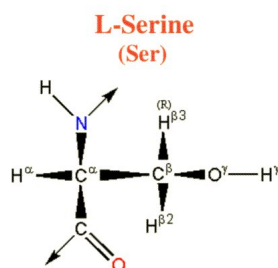
3.63 SER(63)

Figure 53: Image from the BMRB

Residue probability: 0.924

Residue probability confidence: 0.869

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 171.336 | 174.682 | 1.868 | 0.000 | 0.000 |
| CA 3.63.1 | 57.918 | 58.750 | 3.025 | 1.000 | 0.875 |
| CB 3.63.2 | 65.985 | 63.523 | 4.288 | 1.000 | 0.833 |
| N 3.63.3 | 108.104 | 116.135 | 5.326 | 0.917 | 0.917 |
| HA 3.63.4 | 4.986 | 4.486 | 0.430 | 0.778 | 0.875 |
| HB2 3.63.5 | 3.939 | 3.856 | 0.325 | 1.000 | 0.833 |
| HB3 3.63.6 | 4.085 | 3.825 | 0.343 | 0.860 | 0.833 |
| H 3.63.7 | 7.713 | 8.292 | 0.600 | 0.917 | 0.917 |
| HG | NA | – | – | 0.000 | 0.000 |

3.63.1 Detailed Probabilities of SER63CA:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS62 | 1.00 | 1.00 |
| SER63 | 1.00 | 0.80 |
| VAL64 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K62HA | 1.00 |
| S63HB2 | 1.00 |
| S63HB3 | 1.00 |
| S63H | 1.00 |
| S63HG | 1.00 |
| S63HA | 1.00 |
| V64H | 1.00 |
| V64HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS62 | HA | 1.00 | 0.024 | 1.00 | 1.11 |
| LYS62 | HB2 | 0.67 | 0.015 | 1.00 | 0.22 |
| LYS62 | H | 0.87 | 0.005 | 1.00 | 0.09 |
| SER63 | HA | 1.00 | 0.009 | 1.00 | 7.68 |
| SER63 | HB2 | 1.00 | 0.009 | 1.00 | 0.84 |
| SER63 | HB3 | 1.00 | 0.002 | 1.00 | 1.10 |
| SER63 | H | 1.00 | 0.004 | 1.00 | 0.41 |
| VAL64 | HA | 1.00 | 0.013 | 1.00 | 0.27 |
| VAL64 | H | 1.00 | 0.007 | 1.00 | 1.24 |
| VAL64 | HB | 0.52 | 0.021 | 1.00 | 0.28 |

3.63.2 Detailed Probabilities of SER63CB:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER63 | 1.00 | 0.80 |
| VAL64 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S63HA | 1.00 |
| S63HB3 | 1.00 |
| S63H | 1.00 |
| S63HG | 1.00 |
| S63HB2 | 1.00 |
| V64H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER63 | HA | 1.00 | 0.008 | 1.00 | 0.81 |
| SER63 | HB2 | 1.00 | 0.006 | 1.00 | 5.40 |
| SER63 | HB3 | 1.00 | 0.001 | 1.00 | 4.08 |
| SER63 | H | 1.00 | 0.000 | 1.00 | 0.19 |
| VAL64 | H | 1.00 | 0.004 | 1.00 | 0.69 |

3.63.3 Detailed Probabilities of SER63N:

Overall probability: 0.917

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS62 | 0.86 | 1.00 |
| SER63 | 1.00 | 0.80 |
| VAL64 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K62HB2 | 1.00 |
| K62HG2 | 0.97 |
| K62HB3 | 1.00 |
| K62HA | 1.00 |
| K62HG3 | 0.96 |
| K62H | 1.00 |
| S63HA | 1.00 |
| S63HB2 | 1.00 |
| S63HB3 | 1.00 |
| S63HG | 1.00 |
| S63H | 1.00 |
| V64H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS62 | HA | 1.00 | 0.004 | 1.00 | -633644.00 |
| LYS62 | HB2 | 1.00 | 0.001 | 1.00 | -1444562.00 |
| LYS62 | HB3 | 1.00 | 0.080 | 0.00 | 0.00 |
| LYS62 | HG2 | 0.97 | 0.001 | 1.00 | -406648.00 |
| LYS62 | HG3 | 0.96 | 0.009 | 1.00 | -1444562.00 |
| LYS62 | H | 1.00 | 0.001 | 1.00 | -2741988.00 |
| LYS62 | HD3 | 0.60 | 0.019 | 1.00 | -124976.00 |
| SER63 | HA | 1.00 | 0.006 | 1.00 | -957275.00 |
| SER63 | HB2 | 1.00 | 0.004 | 1.00 | -419198.00 |
| SER63 | HB3 | 1.00 | 0.016 | 1.00 | -1449939.00 |
| SER63 | H | 1.00 | 0.001 | 1.00 | -14932196.00 |
| VAL64 | H | 1.00 | 0.001 | 1.00 | -182335.00 |

3.63.4 Detailed Probabilities of SER63HA:

Overall probability: 0.778

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS62 | 0.50 | 1.00 |
| SER63 | 1.00 | 0.80 |
| VAL64 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K62HA | 1.00 |
| S63HB2 | 1.00 |
| S63HB3 | 1.00 |
| S63H | 1.00 |
| S63HG | 1.00 |
| S63HA | 1.00 |
| V64H | 1.00 |
| V64HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS62 | HA | 1.00 | 0.057 | 0.00 | 0.00 |
| LYS62 | H | 0.87 | 0.010 | 1.00 | -113727.00 |
| SER63 | HA | 1.00 | 0.009 | 1.00 | 7.68 |
| SER63 | HB2 | 1.00 | 0.008 | 1.00 | 0.81 |
| SER63 | HB3 | 1.00 | 0.006 | 1.00 | 0.92 |
| SER63 | H | 1.00 | 0.006 | 1.00 | -957275.00 |
| VAL64 | HA | 1.00 | 0.118 | 0.00 | 0.00 |
| VAL64 | H | 1.00 | 0.006 | 1.00 | -1946628.00 |
| VAL64 | HB | 0.52 | 0.009 | 1.00 | 0.13 |

3.63.5 Detailed Probabilities of SER63HB2:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER63 | 1.00 | 0.80 |
| VAL64 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S63HA | 1.00 |
| S63HB3 | 1.00 |
| S63H | 1.00 |
| S63HG | 1.00 |
| S63HB2 | 1.00 |
| V64H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER63 | HA | 1.00 | 0.009 | 1.00 | 0.84 |
| SER63 | HB2 | 1.00 | 0.006 | 1.00 | 5.40 |
| SER63 | HB3 | 1.00 | 0.003 | 1.00 | 3.73 |
| SER63 | H | 1.00 | 0.004 | 1.00 | -419198.00 |
| VAL64 | H | 1.00 | 0.003 | 1.00 | -964557.00 |

3.63.6 Detailed Probabilities of SER63HB3:

Overall probability: 0.860

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER63 | 1.00 | 0.80 |
| VAL64 | 0.30 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S63HA | 1.00 |
| S63HB2 | 1.00 |
| S63H | 1.00 |
| S63HG | 1.00 |
| S63HB3 | 1.00 |
| V64H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER63 | HA | 1.00 | 0.002 | 1.00 | 1.10 |
| SER63 | HB2 | 1.00 | 0.001 | 1.00 | 4.08 |
| SER63 | HB3 | 1.00 | 0.001 | 1.00 | 6.53 |
| SER63 | H | 1.00 | 0.016 | 1.00 | -1449939.00 |
| VAL64 | H | 1.00 | 0.037 | 0.30 | 0.00 |

3.63.7 Detailed Probabilities of SER63H:

Overall probability: 0.917

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS62 | 0.86 | 1.00 |
| SER63 | 1.00 | 0.80 |
| VAL64 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K62HB2 | 1.00 |
| K62HG2 | 0.97 |
| K62HB3 | 1.00 |
| K62HA | 1.00 |
| K62HG3 | 0.96 |
| K62H | 1.00 |
| S63HA | 1.00 |
| S63HB2 | 1.00 |
| S63HB3 | 1.00 |
| S63HG | 1.00 |
| S63H | 1.00 |
| V64H | 1.00 |

NOESY contacts detailed probability

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS62 | HA | 1.00 | 0.002 | 1.00 | 0.40 |
| LYS62 | HB2 | 1.00 | 2.406 | 0.00 | 0.00 |
| LYS62 | HB3 | 1.00 | 0.002 | 1.00 | 0.15 |
| LYS62 | HG2 | 0.97 | 0.010 | 1.00 | 0.10 |
| LYS62 | HG3 | 0.96 | 0.006 | 1.00 | 0.13 |
| LYS62 | H | 1.00 | 0.001 | 1.00 | -1891826.00 |
| LYS62 | HD3 | 0.60 | 0.017 | 1.00 | 0.08 |
| SER63 | HA | 1.00 | 0.004 | 1.00 | 0.41 |
| SER63 | HB2 | 1.00 | 0.000 | 1.00 | 0.19 |
| SER63 | HB3 | 1.00 | 0.000 | 1.00 | 0.19 |
| SER63 | H | 1.00 | 0.001 | 1.00 | -14932196.00 |
| VAL64 | H | 1.00 | 0.001 | 1.00 | -176410.00 |

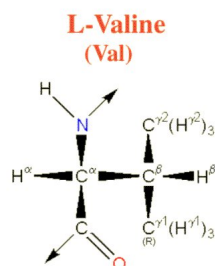
3.64 VAL(64)

Figure 54: Image from the BMRB

Residue probability: 0.844

Residue probability confidence: 0.983

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 171.570 | 175.682 | 2.367 | 0.000 | 0.000 |
| CA 3.64.1 | 60.699 | 62.613 | 4.828 | 0.444 | 1.000 |
| CB 3.64.2 | 36.572 | 32.918 | 4.591 | 1.000 | 1.000 |
| CG1 3.64.3 | 23.329 | 21.563 | 2.746 | 0.857 | 1.000 |
| CG2 3.64.4 | 21.734 | 21.368 | 2.801 | 1.000 | 1.000 |
| N 3.64.5 | 119.063 | 121.057 | 5.832 | 0.840 | 0.917 |
| HA 3.64.6 | 4.760 | 4.178 | 0.599 | 0.750 | 1.000 |
| HB 3.64.7 | 1.675 | 1.980 | 0.322 | 0.833 | 1.000 |
| HG1 3.64.8 | 0.728 | 0.816 | 0.264 | 1.000 | 1.000 |
| HG2 3.64.9 | 0.295 | 0.803 | 0.504 | 0.800 | 1.000 |
| H 3.64.10 | 7.967 | 8.311 | 0.669 | 0.913 | 0.917 |

3.64.1 Detailed Probabilities of VAL64CA:

Overall probability: 0.444

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER63 | 0.00 | 1.00 |
| VAL64 | 0.60 | 1.00 |
| PHE65 | 0.33 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| S63HA | 1.00 |
| V64HG11 | 1.00 |
| V64HG21 | 1.00 |
| V64H | 1.00 |
| V64HB | 1.00 |
| V64HA | 1.00 |
| F65H | 1.00 |
| F65HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER63 | HA | 1.00 | 0.118 | 0.00 | 0.00 |
| VAL64 | HA | 1.00 | 0.344 | 0.00 | 0.00 |
| VAL64 | HB | 1.00 | 0.007 | 1.00 | 0.81 |
| VAL64 | HG11 | 1.00 | 0.014 | 1.00 | 0.24 |
| VAL64 | HG21 | 1.00 | 0.101 | 0.00 | 0.00 |
| VAL64 | H | 1.00 | 0.004 | 1.00 | 0.70 |
| PHE65 | HA | 1.00 | 0.176 | 0.00 | 0.00 |
| PHE65 | H | 1.00 | 0.088 | 0.00 | 0.00 |
| PHE65 | HB2 | 0.52 | 0.014 | 1.00 | 0.72 |

3.64.2 Detailed Probabilities of VAL64CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL64 | 1.00 | 1.00 |
| PHE65 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V64HA | 1.00 |
| V64HG11 | 1.00 |
| V64HG21 | 1.00 |
| V64H | 1.00 |
| V64HB | 1.00 |
| F65H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL64 | HA | 1.00 | 0.020 | 1.00 | 0.30 |
| VAL64 | HB | 1.00 | 0.004 | 1.00 | 5.33 |
| VAL64 | HG11 | 1.00 | 0.003 | 1.00 | 1.40 |
| VAL64 | HG21 | 1.00 | 0.004 | 1.00 | 1.49 |
| VAL64 | H | 1.00 | 0.003 | 1.00 | 0.56 |
| PHE65 | H | 1.00 | 0.010 | 1.00 | 0.10 |

3.64.3 Detailed Probabilities of VAL64CG1:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL64 | 0.80 | 1.00 |
| PHE65 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V64HA | 1.00 |
| V64HG12 | 1.00 |
| V64HG21 | 1.00 |
| V64H | 1.00 |
| V64HB | 1.00 |
| F65H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL64 | HA | 1.00 | 0.016 | 1.00 | 0.91 |
| VAL64 | HB | 1.00 | 0.117 | 0.00 | 0.00 |
| VAL64 | HG11 | 1.00 | 0.004 | 1.00 | 47.71 |
| VAL64 | HG21 | 1.00 | 0.005 | 1.00 | 2.99 |
| VAL64 | H | 1.00 | 0.004 | 1.00 | 0.21 |
| PHE65 | H | 0.98 | 0.006 | 1.00 | 0.68 |
| PHE65 | HA | 0.60 | 0.004 | 1.00 | 0.08 |

3.64.4 Detailed Probabilities of VAL64CG2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL64 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V64HA | 1.00 |
| V64HG11 | 1.00 |
| V64HG22 | 1.00 |
| V64H | 1.00 |
| V64HB | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL64 | HA | 1.00 | 0.016 | 1.00 | 1.01 |
| VAL64 | HB | 1.00 | 0.004 | 1.00 | 1.86 |
| VAL64 | HG11 | 1.00 | 0.002 | 1.00 | 3.40 |
| VAL64 | HG21 | 1.00 | 0.004 | 1.00 | 58.75 |
| VAL64 | H | 1.00 | 0.005 | 1.00 | 0.54 |

3.64.5 Detailed Probabilities of VAL64N:

Overall probability: 0.840

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER63 | 0.83 | 0.80 |
| VAL64 | 1.00 | 1.00 |
| PHE65 | 0.47 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| S63HB3 | 1.00 |
| S63HA | 1.00 |
| S63HB2 | 1.00 |
| S63HG | 0.96 |
| S63H | 1.00 |
| V64HA | 1.00 |
| V64HG11 | 1.00 |
| V64HG21 | 1.00 |
| V64HB | 1.00 |
| V64H | 1.00 |
| F65H | 1.00 |
| F65HA | 0.96 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER63 | HA | 1.00 | 0.006 | 1.00 | -1946628.00 |
| SER63 | HB2 | 1.00 | 0.003 | 1.00 | -964557.00 |
| SER63 | HB3 | 1.00 | 0.037 | 0.30 | 0.00 |
| SER63 | H | 1.00 | 0.001 | 1.00 | -176410.00 |
| VAL64 | HA | 1.00 | 0.017 | 1.00 | -600889.00 |
| VAL64 | HB | 1.00 | 0.000 | 1.00 | -937916.00 |
| VAL64 | HG11 | 1.00 | 0.003 | 1.00 | -487695.00 |
| VAL64 | HG21 | 1.00 | 0.007 | 1.00 | -855998.00 |
| VAL64 | H | 1.00 | 0.018 | 1.00 | -21352072.00 |
| PHE65 | HA | 0.96 | 0.370 | 0.04 | 0.00 |
| PHE65 | H | 1.00 | 0.031 | 0.90 | 0.00 |

3.64.6 Detailed Probabilities of VAL64HA:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER63 | 1.00 | 1.00 |
| VAL64 | 0.80 | 1.00 |
| PHE65 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| S63HA | 1.00 |
| V64HG11 | 1.00 |
| V64HG21 | 1.00 |
| V64H | 1.00 |
| V64HB | 1.00 |
| V64HA | 1.00 |
| F65H | 1.00 |
| F65HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER63 | HA | 1.00 | 0.013 | 1.00 | 0.27 |
| VAL64 | HA | 1.00 | 0.344 | 0.00 | 0.00 |
| VAL64 | HB | 1.00 | 0.020 | 1.00 | 0.30 |
| VAL64 | HG11 | 1.00 | 0.016 | 1.00 | 0.91 |
| VAL64 | HG21 | 1.00 | 0.016 | 1.00 | 1.01 |
| VAL64 | H | 1.00 | 0.017 | 1.00 | -600889.00 |
| PHE65 | HA | 1.00 | 0.063 | 0.00 | 0.00 |
| PHE65 | H | 1.00 | 0.017 | 1.00 | -2852962.00 |

3.64.7 Detailed Probabilities of VAL64HB:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL64 | 0.80 | 1.00 |
| PHE65 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V64HA | 1.00 |
| V64HG11 | 1.00 |
| V64HG21 | 1.00 |
| V64H | 1.00 |
| V64HB | 1.00 |
| F65H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL64 | HA | 1.00 | 0.007 | 1.00 | 0.81 |
| VAL64 | HB | 1.00 | 0.004 | 1.00 | 5.33 |
| VAL64 | HG11 | 1.00 | 0.117 | 0.00 | 0.00 |
| VAL64 | HG21 | 1.00 | 0.004 | 1.00 | 1.86 |
| VAL64 | H | 1.00 | 0.000 | 1.00 | -937916.00 |
| PHE65 | H | 1.00 | 0.003 | 1.00 | -239279.00 |

3.64.8 Detailed Probabilities of VAL64HG11:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL64 | 1.00 | 1.00 |
| PHE65 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V64HA | 1.00 |
| V64HG12 | 1.00 |
| V64HG21 | 1.00 |
| V64H | 1.00 |
| V64HB | 1.00 |
| F65H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL64 | HA | 1.00 | 0.014 | 1.00 | 0.24 |
| VAL64 | HB | 1.00 | 0.003 | 1.00 | 1.40 |
| VAL64 | HG11 | 1.00 | 0.004 | 1.00 | 47.71 |
| VAL64 | HG21 | 1.00 | 0.002 | 1.00 | 3.40 |
| VAL64 | H | 1.00 | 0.003 | 1.00 | -487695.00 |
| PHE65 | H | 0.98 | 0.004 | 1.00 | -1550190.00 |
| PHE65 | HA | 0.60 | 0.016 | 1.00 | 0.15 |

3.64.9 Detailed Probabilities of VAL64HG21:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL64 | 0.80 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V64HA | 1.00 |
| V64HG11 | 1.00 |
| V64HG22 | 1.00 |
| V64H | 1.00 |
| V64HB | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL64 | HA | 1.00 | 0.101 | 0.00 | 0.00 |
| VAL64 | HB | 1.00 | 0.004 | 1.00 | 1.49 |
| VAL64 | HG11 | 1.00 | 0.005 | 1.00 | 2.99 |
| VAL64 | HG21 | 1.00 | 0.004 | 1.00 | 58.75 |
| VAL64 | H | 1.00 | 0.007 | 1.00 | -855998.00 |

3.64.10 Detailed Probabilities of VAL64H:

Overall probability: 0.913

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER63 | 1.00 | 0.80 |
| VAL64 | 1.00 | 1.00 |
| PHE65 | 0.52 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| S63HB3 | 1.00 |
| S63HA | 1.00 |
| S63HB2 | 1.00 |
| S63HG | 0.96 |
| S63H | 1.00 |
| V64HA | 1.00 |
| V64HG11 | 1.00 |
| V64HG21 | 1.00 |
| V64HB | 1.00 |
| V64H | 1.00 |
| F65H | 1.00 |
| F65HA | 0.96 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER63 | HA | 1.00 | 0.007 | 1.00 | 1.24 |
| SER63 | HB2 | 1.00 | 0.004 | 1.00 | 0.69 |
| SER63 | HB3 | 1.00 | 0.003 | 1.00 | 0.55 |
| SER63 | H | 1.00 | 0.001 | 1.00 | -182335.00 |
| VAL64 | HA | 1.00 | 0.004 | 1.00 | 0.70 |
| VAL64 | HB | 1.00 | 0.003 | 1.00 | 0.56 |
| VAL64 | HG11 | 1.00 | 0.004 | 1.00 | 0.21 |
| VAL64 | HG21 | 1.00 | 0.005 | 1.00 | 0.54 |
| VAL64 | H | 1.00 | 0.018 | 1.00 | -21352072.00 |
| PHE65 | HA | 0.96 | 0.410 | 0.04 | 0.00 |
| PHE65 | H | 1.00 | 0.002 | 1.00 | -163578.00 |

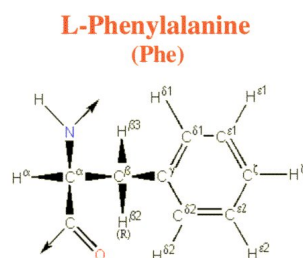
3.65 PHE(65)

Figure 55: Image from the BMRB

Residue probability: 0.528

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 174.612 | 175.508 | 2.010 | 0.000 | 0.000 |
| CA 3.65.1 | 56.425 | 58.245 | 3.808 | 0.753 | 1.000 |
| CB 3.65.2 | 42.896 | 40.078 | 3.616 | 0.823 | 1.000 |
| CD1 3.65.3 | 131.911 | 131.234 | 9.579 | 0.644 | 1.000 |
| CD2 3.65.4 | 131.960 | 131.352 | 9.581 | 0.646 | 1.000 |
| CE1 3.65.5 | 130.694 | 130.599 | 3.219 | 0.000 | 1.000 |
| CE2 3.65.6 | 131.063 | 130.633 | 2.839 | 0.001 | 1.000 |
| CZ 3.65.7 | 129.603 | 129.042 | 3.448 | 0.000 | 1.000 |
| N 3.65.8 | 126.034 | 120.315 | 4.931 | 1.000 | 1.000 |
| HA 3.65.9 | 5.350 | 4.625 | 1.237 | 0.640 | 1.000 |
| HB2 3.65.10 | 3.232 | 2.980 | 0.399 | 0.778 | 1.000 |
| HB3 3.65.11 | 3.037 | 2.916 | 0.434 | 0.750 | 1.000 |
| HD1 3.65.12 | 7.254 | 7.037 | 0.347 | 0.667 | 1.000 |
| HD2 3.65.13 | 7.254 | 7.022 | 0.417 | 0.667 | 1.000 |
| HE1 3.65.14 | 7.286 | 7.046 | 0.417 | 0.350 | 1.000 |
| HE2 3.65.15 | 7.286 | 7.043 | 0.400 | 0.200 | 1.000 |
| HZ 3.65.16 | 7.272 | 6.984 | 1.598 | 0.320 | 1.000 |
| H 3.65.17 | 9.082 | 8.375 | 0.710 | 0.743 | 1.000 |

3.65.1 Detailed Probabilities of PHE65CA:

Overall probability: 0.753

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL64 | 0.35 | 1.00 |
| PHE65 | 1.00 | 1.00 |
| PHE66 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| V64HA | 1.00 |
| V64H | 0.96 |
| F65HB2 | 1.00 |
| F65HB3 | 1.00 |
| F65HD1 | 1.00 |
| F65HD2 | 1.00 |
| F65H | 1.00 |
| F65HA | 1.00 |
| F66HA | 1.00 |
| F66H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL64 | HA | 1.00 | 0.063 | 0.00 | 0.00 |
| VAL64 | H | 0.96 | 0.410 | 0.04 | 0.00 |
| VAL64 | HG11 | 0.61 | 0.016 | 1.00 | 0.15 |
| PHE65 | HA | 1.00 | 0.006 | 1.00 | 2.08 |
| PHE65 | HB2 | 1.00 | 0.002 | 1.00 | 0.38 |
| PHE65 | HB3 | 1.00 | 0.005 | 1.00 | 0.23 |
| PHE65 | HD1 | 1.00 | 0.004 | 1.00 | 0.23 |
| PHE65 | HD2 | 1.00 | 0.004 | 1.00 | 0.23 |
| PHE65 | H | 1.00 | 0.003 | 1.00 | 0.17 |
| PHE65 | HE1 | 0.74 | 0.028 | 1.00 | 0.23 |
| PHE66 | HA | 1.00 | 0.163 | 0.00 | 0.00 |
| PHE66 | H | 1.00 | 0.005 | 1.00 | 0.80 |

3.65.2 Detailed Probabilities of PHE65CB:

Overall probability: 0.823

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE65 | 0.80 | 1.00 |
| PHE66 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F65HA | 1.00 |
| F65HB3 | 1.00 |
| F65HD1 | 1.00 |
| F65HD2 | 1.00 |
| F65HE2 | 1.00 |
| F65H | 1.00 |
| F65HB2 | 1.00 |
| F66H | 1.00 |

NOESY contacts detailed probability

3.65 PHE(65)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE65 | HA | 1.00 | 0.007 | 1.00 | 0.42 |
| PHE65 | HB2 | 1.00 | 0.201 | 0.00 | 0.00 |
| PHE65 | HB3 | 1.00 | 0.006 | 1.00 | 1.52 |
| PHE65 | HD1 | 1.00 | 0.003 | 1.00 | 0.62 |
| PHE65 | HD2 | 1.00 | 0.003 | 1.00 | 0.62 |
| PHE65 | HE2 | 1.00 | 0.035 | 0.50 | 0.00 |
| PHE65 | H | 1.00 | 0.009 | 1.00 | 0.33 |
| PHE65 | HE1 | 0.90 | 0.035 | 0.90 | 0.00 |
| PHE66 | H | 1.00 | 0.006 | 1.00 | 0.12 |

3.65.3 Detailed Probabilities of PHE65CD1:

Overall probability: 0.644

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE65 | 0.64 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F65HA | 1.00 |
| F65HB2 | 1.00 |
| F65HB3 | 1.00 |
| F65HD2 | 1.00 |
| F65HE1 | 1.00 |
| F65HE2 | 1.00 |
| F65HZ | 1.00 |
| F65H | 1.00 |
| F65HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE65 | HA | 1.00 | 0.015 | 1.00 | 0.44 |
| PHE65 | HB2 | 1.00 | 0.001 | 1.00 | 0.81 |
| PHE65 | HB3 | 1.00 | 0.014 | 1.00 | 0.80 |
| PHE65 | HD1 | 1.00 | 0.014 | 1.00 | 27.85 |
| PHE65 | HD2 | 1.00 | 0.014 | 1.00 | 27.85 |
| PHE65 | HE1 | 1.00 | 0.046 | 0.00 | 0.00 |
| PHE65 | HE2 | 1.00 | 0.046 | 0.00 | 0.00 |
| PHE65 | HZ | 1.00 | 0.032 | 0.80 | 0.00 |
| PHE65 | H | 1.00 | 0.242 | 0.00 | 0.00 |

3.65.4 Detailed Probabilities of PHE65CD2:

Overall probability: 0.646

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE65 | 0.65 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F65HA | 1.00 |
| F65HB2 | 1.00 |
| F65HB3 | 1.00 |
| F65HD1 | 1.00 |
| F65HE1 | 1.00 |
| F65HE2 | 1.00 |
| F65HZ | 1.00 |
| F65H | 0.99 |
| F65HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE65 | HA | 1.00 | 0.015 | 1.00 | 0.44 |
| PHE65 | HB2 | 1.00 | 0.001 | 1.00 | 0.81 |
| PHE65 | HB3 | 1.00 | 0.014 | 1.00 | 0.80 |
| PHE65 | HD1 | 1.00 | 0.014 | 1.00 | 27.85 |
| PHE65 | HD2 | 1.00 | 0.014 | 1.00 | 27.85 |
| PHE65 | HE1 | 1.00 | 0.046 | 0.00 | 0.00 |
| PHE65 | HE2 | 1.00 | 0.046 | 0.00 | 0.00 |
| PHE65 | HZ | 1.00 | 0.032 | 0.80 | 0.00 |
| PHE65 | H | 0.99 | 0.242 | 0.01 | 0.00 |

3.65.5 Detailed Probabilities of PHE65CE1:

Overall probability: 0.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE65 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F65HD1 | 1.00 |
| F65HD2 | 1.00 |
| F65HE2 | 1.00 |
| F65HZ | 1.00 |
| F65HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE65 | HD1 | 1.00 | 1.542 | 0.00 | 0.00 |
| PHE65 | HD2 | 1.00 | 1.542 | 0.00 | 0.00 |
| PHE65 | HE1 | 1.00 | 1.574 | 0.00 | 0.00 |
| PHE65 | HE2 | 1.00 | 1.574 | 0.00 | 0.00 |
| PHE65 | HZ | 1.00 | 1.560 | 0.00 | 0.00 |

3.65.6 Detailed Probabilities of PHE65CE2:

Overall probability: 0.001

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE65 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F65HB2 | 1.00 |
| F65HB3 | 1.00 |
| F65HD1 | 1.00 |
| F65HD2 | 1.00 |
| F65HE1 | 1.00 |
| F65HZ | 1.00 |
| F65HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE65 | HB2 | 1.00 | 0.658 | 0.00 | 0.00 |
| PHE65 | HB3 | 1.00 | 0.463 | 0.00 | 0.00 |
| PHE65 | HD1 | 1.00 | 1.542 | 0.00 | 0.00 |
| PHE65 | HD2 | 1.00 | 1.542 | 0.00 | 0.00 |
| PHE65 | HE1 | 1.00 | 1.574 | 0.00 | 0.00 |
| PHE65 | HE2 | 1.00 | 1.574 | 0.00 | 0.00 |
| PHE65 | HZ | 1.00 | 1.560 | 0.00 | 0.00 |

3.65.7 Detailed Probabilities of PHE65CZ:

Overall probability: 0.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE65 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F65HD1 | 1.00 |
| F65HD2 | 1.00 |
| F65HE1 | 1.00 |
| F65HE2 | 1.00 |
| F65HZ | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE65 | HD1 | 1.00 | 0.082 | 0.00 | 0.00 |
| PHE65 | HD2 | 1.00 | 0.082 | 0.00 | 0.00 |
| PHE65 | HE1 | 1.00 | 0.114 | 0.00 | 0.00 |
| PHE65 | HE2 | 1.00 | 0.114 | 0.00 | 0.00 |
| PHE65 | HZ | 1.00 | 0.100 | 0.00 | 0.00 |

3.65.8 Detailed Probabilities of PHE65N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL64 | 1.00 | 1.00 |
| PHE65 | 1.00 | 1.00 |
| PHE66 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V64H | 1.00 |
| V64HG13 | 0.98 |
| V64HB | 1.00 |
| V64HA | 1.00 |
| F65HA | 1.00 |
| F65HB2 | 1.00 |
| F65HB3 | 1.00 |
| F65HD1 | 1.00 |
| F65HD2 | 0.99 |
| F65H | 1.00 |
| F66H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL64 | HA | 1.00 | 0.017 | 1.00 | -2852962.00 |
| VAL64 | HB | 1.00 | 0.003 | 1.00 | -239279.00 |
| VAL64 | HG11 | 0.98 | 0.004 | 1.00 | -1550190.00 |
| VAL64 | H | 1.00 | 0.002 | 1.00 | -163578.00 |
| VAL64 | HG21 | 0.95 | 0.006 | 1.00 | -473537.00 |
| PHE65 | HA | 1.00 | 0.007 | 1.00 | -542943.00 |
| PHE65 | HB2 | 1.00 | 0.003 | 1.00 | -671863.00 |
| PHE65 | HB3 | 1.00 | 0.011 | 1.00 | -834612.00 |
| PHE65 | HD1 | 1.00 | 0.006 | 1.00 | -213499.00 |
| PHE65 | HD2 | 0.99 | 0.006 | 1.00 | -213499.00 |
| PHE65 | H | 1.00 | 0.007 | 1.00 | -9750638.00 |
| PHE66 | H | 1.00 | 0.005 | 1.00 | -170848.00 |
| PHE66 | HB2 | 0.56 | 0.024 | 1.00 | -671863.00 |

3.65.9 Detailed Probabilities of PHE65HA:

Overall probability: 0.640

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL64 | 0.35 | 1.00 |
| PHE65 | 0.83 | 1.00 |
| PHE66 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| V64HA | 1.00 |
| V64H | 0.96 |
| F65HB2 | 1.00 |
| F65HB3 | 1.00 |
| F65HD1 | 1.00 |
| F65HD2 | 1.00 |
| F65H | 1.00 |
| F65HA | 1.00 |
| F66HA | 1.00 |
| F66H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL64 | HA | 1.00 | 0.176 | 0.00 | 0.00 |
| VAL64 | H | 0.96 | 0.370 | 0.04 | 0.00 |
| VAL64 | HG11 | 0.61 | 0.004 | 1.00 | 0.08 |
| PHE65 | HA | 1.00 | 0.006 | 1.00 | 2.08 |
| PHE65 | HB2 | 1.00 | 0.007 | 1.00 | 0.42 |
| PHE65 | HB3 | 1.00 | 0.151 | 0.00 | 0.00 |
| PHE65 | HD1 | 1.00 | 0.015 | 1.00 | 0.44 |
| PHE65 | HD2 | 1.00 | 0.015 | 1.00 | 0.44 |
| PHE65 | H | 1.00 | 0.007 | 1.00 | -542943.00 |
| PHE66 | HA | 1.00 | 0.052 | 0.00 | 0.00 |
| PHE66 | H | 1.00 | 0.008 | 1.00 | -1827001.00 |

3.65.10 Detailed Probabilities of PHE65HB2:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE65 | 0.71 | 1.00 |
| PHE66 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F65HA | 1.00 |
| F65HB3 | 1.00 |
| F65HD1 | 1.00 |
| F65HD2 | 1.00 |
| F65HE2 | 1.00 |
| F65H | 1.00 |
| F65HB2 | 1.00 |
| F66H | 1.00 |

NOESY contacts detailed probability

3.65 PHE(65)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE65 | HA | 1.00 | 0.002 | 1.00 | 0.38 |
| PHE65 | HB2 | 1.00 | 0.201 | 0.00 | 0.00 |
| PHE65 | HB3 | 1.00 | 0.001 | 1.00 | 1.33 |
| PHE65 | HD1 | 1.00 | 0.001 | 1.00 | 0.81 |
| PHE65 | HD2 | 1.00 | 0.001 | 1.00 | 0.81 |
| PHE65 | HE2 | 1.00 | 0.658 | 0.00 | 0.00 |
| PHE65 | H | 1.00 | 0.003 | 1.00 | -671863.00 |
| PHE66 | H | 1.00 | 0.015 | 1.00 | -718077.00 |
| PHE66 | HA | 0.59 | 0.017 | 1.00 | 0.46 |

3.65.11 Detailed Probabilities of PHE65HB3:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE65 | 0.71 | 1.00 |
| PHE66 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F65HA | 1.00 |
| F65HB2 | 1.00 |
| F65HD1 | 1.00 |
| F65HD2 | 1.00 |
| F65HE2 | 1.00 |
| F65H | 1.00 |
| F65HB3 | 1.00 |
| F66H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE65 | HA | 1.00 | 0.005 | 1.00 | 0.23 |
| PHE65 | HB2 | 1.00 | 0.006 | 1.00 | 1.52 |
| PHE65 | HB3 | 1.00 | 0.196 | 0.00 | 0.00 |
| PHE65 | HD1 | 1.00 | 0.014 | 1.00 | 0.80 |
| PHE65 | HD2 | 1.00 | 0.014 | 1.00 | 0.80 |
| PHE65 | HE2 | 1.00 | 0.463 | 0.00 | 0.00 |
| PHE65 | H | 1.00 | 0.011 | 1.00 | -834612.00 |
| PHE66 | H | 1.00 | 0.010 | 1.00 | -153150.00 |

3.65.12 Detailed Probabilities of PHE65HD1:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE65 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F65HA | 1.00 |
| F65HB2 | 1.00 |
| F65HB3 | 1.00 |
| F65HD2 | 1.00 |
| F65HE1 | 1.00 |
| F65HE2 | 1.00 |
| F65HZ | 1.00 |
| F65H | 1.00 |
| F65HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE65 | HA | 1.00 | 0.004 | 1.00 | 0.23 |
| PHE65 | HB2 | 1.00 | 0.003 | 1.00 | 0.62 |
| PHE65 | HB3 | 1.00 | 0.001 | 1.00 | 0.41 |
| PHE65 | HD1 | 1.00 | 0.014 | 1.00 | 27.85 |
| PHE65 | HD2 | 1.00 | 0.014 | 1.00 | 27.85 |
| PHE65 | HE1 | 1.00 | 1.542 | 0.00 | 0.00 |
| PHE65 | HE2 | 1.00 | 1.542 | 0.00 | 0.00 |
| PHE65 | HZ | 1.00 | 0.082 | 0.00 | 0.00 |
| PHE65 | H | 1.00 | 0.006 | 1.00 | -213499.00 |

3.65.13 Detailed Probabilities of PHE65HD2:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE65 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F65HA | 1.00 |
| F65HB2 | 1.00 |
| F65HB3 | 1.00 |
| F65HD1 | 1.00 |
| F65HE1 | 1.00 |
| F65HE2 | 1.00 |
| F65HZ | 1.00 |
| F65H | 0.99 |
| F65HD2 | 1.00 |

NOESY contacts detailed probability

3.65 PHE(65)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE65 | HA | 1.00 | 0.004 | 1.00 | 0.23 |
| PHE65 | HB2 | 1.00 | 0.003 | 1.00 | 0.62 |
| PHE65 | HB3 | 1.00 | 0.001 | 1.00 | 0.41 |
| PHE65 | HD1 | 1.00 | 0.014 | 1.00 | 27.85 |
| PHE65 | HD2 | 1.00 | 0.014 | 1.00 | 27.85 |
| PHE65 | HE1 | 1.00 | 1.542 | 0.00 | 0.00 |
| PHE65 | HE2 | 1.00 | 1.542 | 0.00 | 0.00 |
| PHE65 | HZ | 1.00 | 0.082 | 0.00 | 0.00 |
| PHE65 | H | 0.99 | 0.006 | 1.00 | -213499.00 |

3.65.14 Detailed Probabilities of PHE65HE1:

Overall probability: 0.350

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE65 | 0.35 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F65HD1 | 1.00 |
| F65HD2 | 1.00 |
| F65HE2 | 1.00 |
| F65HZ | 1.00 |
| F65HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE65 | HD1 | 1.00 | 0.046 | 0.00 | 0.00 |
| PHE65 | HD2 | 1.00 | 0.046 | 0.00 | 0.00 |
| PHE65 | HE1 | 1.00 | 1.574 | 0.00 | 0.00 |
| PHE65 | HE2 | 1.00 | 1.574 | 0.00 | 0.00 |
| PHE65 | HZ | 1.00 | 0.114 | 0.00 | 0.00 |
| PHE65 | HA | 0.74 | 0.028 | 1.00 | 0.23 |
| PHE65 | HB2 | 0.90 | 0.035 | 0.90 | 0.00 |
| PHE65 | HB3 | 0.89 | 0.031 | 0.90 | 0.00 |

3.65.15 Detailed Probabilities of PHE65HE2:

Overall probability: 0.200

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE65 | 0.20 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F65HB2 | 1.00 |
| F65HB3 | 1.00 |
| F65HD1 | 1.00 |
| F65HD2 | 1.00 |
| F65HE1 | 1.00 |
| F65HZ | 1.00 |
| F65HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE65 | HB2 | 1.00 | 0.035 | 0.50 | 0.00 |
| PHE65 | HB3 | 1.00 | 0.031 | 0.90 | 0.00 |
| PHE65 | HD1 | 1.00 | 0.046 | 0.00 | 0.00 |
| PHE65 | HD2 | 1.00 | 0.046 | 0.00 | 0.00 |
| PHE65 | HE1 | 1.00 | 1.574 | 0.00 | 0.00 |
| PHE65 | HE2 | 1.00 | 1.574 | 0.00 | 0.00 |
| PHE65 | HZ | 1.00 | 0.114 | 0.00 | 0.00 |

3.65.16 Detailed Probabilities of PHE65HZ:

Overall probability: 0.320

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE65 | 0.32 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F65HD1 | 1.00 |
| F65HD2 | 1.00 |
| F65HE1 | 1.00 |
| F65HE2 | 1.00 |
| F65HZ | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE65 | HD1 | 1.00 | 0.032 | 0.80 | 0.00 |
| PHE65 | HD2 | 1.00 | 0.032 | 0.80 | 0.00 |
| PHE65 | HE1 | 1.00 | 1.560 | 0.00 | 0.00 |
| PHE65 | HE2 | 1.00 | 1.560 | 0.00 | 0.00 |
| PHE65 | HZ | 1.00 | 0.100 | 0.00 | 0.00 |

3.65.17 Detailed Probabilities of PHE65H:

Overall probability: 0.743

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL64 | 0.78 | 1.00 |
| PHE65 | 0.67 | 1.00 |
| PHE66 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V64H | 1.00 |
| V64HG13 | 0.98 |
| V64HB | 1.00 |
| V64HA | 1.00 |
| F65HA | 1.00 |
| F65HB2 | 1.00 |
| F65HB3 | 1.00 |
| F65HD1 | 1.00 |
| F65HD2 | 0.99 |
| F65H | 1.00 |
| F66H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL64 | HA | 1.00 | 0.088 | 0.00 | 0.00 |
| VAL64 | HB | 1.00 | 0.010 | 1.00 | 0.10 |
| VAL64 | HG11 | 0.98 | 0.006 | 1.00 | 0.68 |
| VAL64 | H | 1.00 | 0.031 | 0.90 | 0.00 |
| VAL64 | HG21 | 0.95 | 0.016 | 1.00 | 0.23 |
| PHE65 | HA | 1.00 | 0.003 | 1.00 | 0.17 |
| PHE65 | HB2 | 1.00 | 0.009 | 1.00 | 0.33 |
| PHE65 | HB3 | 1.00 | 0.009 | 1.00 | 0.32 |
| PHE65 | HD1 | 1.00 | 0.242 | 0.00 | 0.00 |
| PHE65 | HD2 | 0.99 | 0.242 | 0.01 | 0.00 |
| PHE65 | H | 1.00 | 0.007 | 1.00 | -9750638.00 |
| PHE66 | H | 1.00 | 0.004 | 1.00 | -117557.00 |

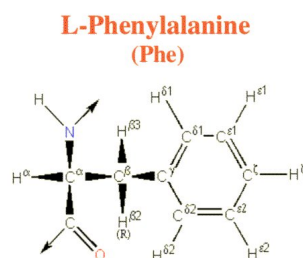
3.66 PHE(66)

Figure 56: Image from the BMRB

Residue probability: 0.922

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 173.546 | 175.508 | 2.010 | 0.000 | 0.000 |
| CA 3.66.1 | 52.709 | 58.245 | 3.808 | 0.833 | 1.000 |
| CB 3.66.2 | 39.595 | 40.078 | 3.616 | 0.875 | 1.000 |
| CD1 3.66.3 | 128.988 | 131.234 | 9.579 | 1.000 | 1.000 |
| CD2 3.66.4 | 129.118 | 131.352 | 9.581 | 1.000 | 1.000 |
| CE1 3.66.5 | 131.093 | 130.599 | 3.219 | 1.000 | 1.000 |
| CE2 3.66.6 | 131.275 | 130.633 | 2.839 | 0.857 | 1.000 |
| CZ 3.66.7 | 128.420 | 129.042 | 3.448 | 1.000 | 1.000 |
| N 3.66.8 | 127.185 | 120.315 | 4.931 | 1.000 | 1.000 |
| HA 3.66.9 | 5.507 | 4.625 | 1.237 | 0.909 | 1.000 |
| HB2 3.66.10 | 3.205 | 2.980 | 0.399 | 0.900 | 1.000 |
| HB3 3.66.11 | 3.336 | 2.916 | 0.434 | 0.875 | 1.000 |
| HD1 3.66.12 | 7.148 | 7.037 | 0.347 | 0.889 | 1.000 |
| HD2 3.66.13 | 7.148 | 7.022 | 0.417 | 0.889 | 1.000 |
| HE1 3.66.14 | 6.953 | 7.046 | 0.417 | 1.000 | 1.000 |
| HE2 3.66.15 | 6.953 | 7.043 | 0.400 | 0.715 | 1.000 |
| HZ 3.66.16 | 6.625 | 6.984 | 1.598 | 1.000 | 1.000 |
| H 3.66.17 | 9.313 | 8.375 | 0.710 | 0.929 | 1.000 |

3.66.1 Detailed Probabilities of PHE66CA:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE65 | 0.50 | 1.00 |
| PHE66 | 1.00 | 1.00 |
| GLY67 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F65HA | 1.00 |
| F66HB2 | 1.00 |
| F66HB3 | 1.00 |
| F66HD1 | 1.00 |
| F66HD2 | 1.00 |
| F66H | 1.00 |
| F66HA | 1.00 |
| G67H | 1.00 |
| G67HA2 | 1.00 |
| G67HA3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE65 | HA | 1.00 | 0.052 | 0.00 | 0.00 |
| PHE65 | HB2 | 0.59 | 0.017 | 1.00 | 0.46 |
| PHE66 | HA | 1.00 | 0.005 | 1.00 | 3.13 |
| PHE66 | HB2 | 1.00 | 0.010 | 1.00 | 0.46 |
| PHE66 | HB3 | 1.00 | 0.007 | 1.00 | 0.22 |
| PHE66 | HD1 | 1.00 | 0.004 | 1.00 | 0.66 |
| PHE66 | HD2 | 1.00 | 0.004 | 1.00 | 0.66 |
| PHE66 | H | 1.00 | 0.016 | 1.00 | 0.14 |
| PHE66 | HE1 | 0.74 | 0.006 | 1.00 | 0.14 |
| GLY67 | HA2 | 1.00 | 0.557 | 0.00 | 0.00 |
| GLY67 | HA3 | 1.00 | 0.015 | 1.00 | 0.09 |
| GLY67 | H | 1.00 | 0.006 | 1.00 | 0.79 |

3.66.2 Detailed Probabilities of PHE66CB:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE66 | 0.86 | 1.00 |
| GLY67 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F66HA | 1.00 |
| F66HB2 | 1.00 |
| F66HD1 | 1.00 |
| F66HD2 | 1.00 |
| F66HE2 | 1.00 |
| F66H | 1.00 |
| F66HB3 | 1.00 |
| G67H | 1.00 |

NOESY contacts detailed probability

3.66 PHE(66)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE66 | HA | 1.00 | 0.003 | 1.00 | 0.17 |
| PHE66 | HB2 | 1.00 | 0.007 | 1.00 | 0.88 |
| PHE66 | HB3 | 1.00 | 0.007 | 1.00 | 0.87 |
| PHE66 | HD1 | 1.00 | 0.004 | 1.00 | 0.18 |
| PHE66 | HD2 | 1.00 | 0.004 | 1.00 | 0.18 |
| PHE66 | HE2 | 1.00 | 0.199 | 0.00 | 0.00 |
| PHE66 | H | 1.00 | 0.004 | 1.00 | 0.17 |
| GLY67 | H | 1.00 | 0.010 | 1.00 | 0.08 |

3.66.3 Detailed Probabilities of PHE66CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE66 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F66HA | 1.00 |
| F66HB2 | 1.00 |
| F66HB3 | 1.00 |
| F66HD2 | 1.00 |
| F66HE1 | 1.00 |
| F66HE2 | 1.00 |
| F66HZ | 1.00 |
| F66H | 1.00 |
| F66HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE66 | HA | 1.00 | 0.002 | 1.00 | 0.36 |
| PHE66 | HB2 | 1.00 | 0.005 | 1.00 | 0.83 |
| PHE66 | HB3 | 1.00 | 0.004 | 1.00 | 0.17 |
| PHE66 | HD1 | 1.00 | 0.004 | 1.00 | 27.71 |
| PHE66 | HD2 | 1.00 | 0.004 | 1.00 | 27.71 |
| PHE66 | HE1 | 1.00 | 0.005 | 1.00 | 2.23 |
| PHE66 | HE2 | 1.00 | 0.005 | 1.00 | 2.23 |
| PHE66 | HZ | 1.00 | 0.010 | 1.00 | 0.60 |
| PHE66 | H | 1.00 | 0.001 | 1.00 | 0.18 |

3.66.4 Detailed Probabilities of PHE66CD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE66 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F66HA | 1.00 |
| F66HB2 | 1.00 |
| F66HB3 | 1.00 |
| F66HD1 | 1.00 |
| F66HE1 | 1.00 |
| F66HE2 | 1.00 |
| F66HZ | 1.00 |
| F66H | 0.99 |
| F66HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE66 | HA | 1.00 | 0.002 | 1.00 | 0.36 |
| PHE66 | HB2 | 1.00 | 0.005 | 1.00 | 0.83 |
| PHE66 | HB3 | 1.00 | 0.004 | 1.00 | 0.17 |
| PHE66 | HD1 | 1.00 | 0.004 | 1.00 | 27.71 |
| PHE66 | HD2 | 1.00 | 0.004 | 1.00 | 27.71 |
| PHE66 | HE1 | 1.00 | 0.005 | 1.00 | 2.23 |
| PHE66 | HE2 | 1.00 | 0.005 | 1.00 | 2.23 |
| PHE66 | HZ | 1.00 | 0.010 | 1.00 | 0.60 |
| PHE66 | H | 0.99 | 0.001 | 1.00 | 0.18 |

3.66.5 Detailed Probabilities of PHE66CE1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE66 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F66HD1 | 1.00 |
| F66HD2 | 1.00 |
| F66HE2 | 1.00 |
| F66HZ | 1.00 |
| F66HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE66 | HD1 | 1.00 | 0.001 | 1.00 | 8.45 |
| PHE66 | HD2 | 1.00 | 0.001 | 1.00 | 8.45 |
| PHE66 | HE1 | 1.00 | 0.004 | 1.00 | 6.93 |
| PHE66 | HE2 | 1.00 | 0.004 | 1.00 | 6.93 |
| PHE66 | HZ | 1.00 | 0.002 | 1.00 | 2.37 |
| PHE66 | HA | 0.74 | 0.004 | 1.00 | 0.08 |
| PHE66 | HB2 | 0.90 | 0.011 | 1.00 | 0.09 |

3.66.6 Detailed Probabilities of PHE66CE2:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE66 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F66HB2 | 1.00 |
| F66HB3 | 1.00 |
| F66HD1 | 1.00 |
| F66HD2 | 1.00 |
| F66HE1 | 1.00 |
| F66HZ | 1.00 |
| F66HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE66 | HB2 | 1.00 | 0.011 | 1.00 | 0.09 |
| PHE66 | HB3 | 1.00 | 0.108 | 0.00 | 0.00 |
| PHE66 | HD1 | 1.00 | 0.001 | 1.00 | 8.45 |
| PHE66 | HD2 | 1.00 | 0.001 | 1.00 | 8.45 |
| PHE66 | HE1 | 1.00 | 0.004 | 1.00 | 6.93 |
| PHE66 | HE2 | 1.00 | 0.004 | 1.00 | 6.93 |
| PHE66 | HZ | 1.00 | 0.002 | 1.00 | 2.37 |

3.66.7 Detailed Probabilities of PHE66CZ:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE66 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F66HD1 | 1.00 |
| F66HD2 | 1.00 |
| F66HE1 | 1.00 |
| F66HE2 | 1.00 |
| F66HZ | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE66 | HD1 | 1.00 | 0.004 | 1.00 | 0.10 |
| PHE66 | HD2 | 1.00 | 0.004 | 1.00 | 0.10 |
| PHE66 | HE1 | 1.00 | 0.001 | 1.00 | 1.66 |
| PHE66 | HE2 | 1.00 | 0.001 | 1.00 | 1.66 |
| PHE66 | HZ | 1.00 | 0.002 | 1.00 | 2.55 |

3.66.8 Detailed Probabilities of PHE66N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE65 | 1.00 | 1.00 |
| PHE66 | 1.00 | 1.00 |
| GLY67 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F65HB3 | 1.00 |
| F65HB2 | 1.00 |
| F65HA | 1.00 |
| F65H | 1.00 |
| F66HA | 1.00 |
| F66HB2 | 1.00 |
| F66HB3 | 1.00 |
| F66HD1 | 1.00 |
| F66HD2 | 0.99 |
| F66H | 1.00 |
| G67H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE65 | HA | 1.00 | 0.008 | 1.00 | -1827001.00 |
| PHE65 | HB2 | 1.00 | 0.015 | 1.00 | -718077.00 |
| PHE65 | HB3 | 1.00 | 0.010 | 1.00 | -153150.00 |
| PHE65 | H | 1.00 | 0.004 | 1.00 | -117557.00 |
| PHE65 | HD1 | 0.79 | 0.005 | 1.00 | -250298.00 |
| PHE65 | HD2 | 0.70 | 0.005 | 1.00 | -250298.00 |
| PHE66 | HA | 1.00 | 0.005 | 1.00 | -399647.00 |
| PHE66 | HB2 | 1.00 | 0.012 | 1.00 | -718077.00 |
| PHE66 | HB3 | 1.00 | 0.007 | 1.00 | -725670.00 |
| PHE66 | HD1 | 1.00 | 0.005 | 1.00 | -280148.00 |
| PHE66 | HD2 | 0.99 | 0.005 | 1.00 | -280148.00 |
| PHE66 | H | 1.00 | 0.006 | 1.00 | -6412614.00 |
| GLY67 | H | 1.00 | 0.004 | 1.00 | -104371.00 |

3.66.9 Detailed Probabilities of PHE66HA:

Overall probability: 0.909

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE65 | 0.00 | 1.00 |
| PHE66 | 1.00 | 1.00 |
| GLY67 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F65HA | 1.00 |
| F66HB2 | 1.00 |
| F66HB3 | 1.00 |
| F66HD1 | 1.00 |
| F66HD2 | 1.00 |
| F66H | 1.00 |
| F66HA | 1.00 |
| G67H | 1.00 |
| G67HA2 | 1.00 |
| G67HA3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE65 | HA | 1.00 | 0.163 | 0.00 | 0.00 |
| PHE66 | HA | 1.00 | 0.005 | 1.00 | 3.13 |
| PHE66 | HB2 | 1.00 | 0.004 | 1.00 | 0.20 |
| PHE66 | HB3 | 1.00 | 0.003 | 1.00 | 0.17 |
| PHE66 | HD1 | 1.00 | 0.002 | 1.00 | 0.36 |
| PHE66 | HD2 | 1.00 | 0.002 | 1.00 | 0.36 |
| PHE66 | H | 1.00 | 0.005 | 1.00 | -399647.00 |
| PHE66 | HE1 | 0.74 | 0.004 | 1.00 | 0.08 |
| GLY67 | HA2 | 1.00 | 0.019 | 1.00 | 0.08 |
| GLY67 | HA3 | 1.00 | 0.002 | 1.00 | 0.48 |
| GLY67 | H | 1.00 | 0.001 | 1.00 | -2343828.00 |

3.66.10 Detailed Probabilities of PHE66HB2:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE66 | 0.88 | 1.00 |
| GLY67 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F66HA | 1.00 |
| F66HB3 | 1.00 |
| F66HD1 | 1.00 |
| F66HD2 | 1.00 |
| F66HE2 | 1.00 |
| F66H | 1.00 |
| F66HB2 | 1.00 |
| G67H | 1.00 |

NOESY contacts detailed probability

3.66 PHE(66)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE66 | HA | 1.00 | 0.010 | 1.00 | 0.46 |
| PHE66 | HB2 | 1.00 | 0.125 | 0.00 | 0.00 |
| PHE66 | HB3 | 1.00 | 0.007 | 1.00 | 0.88 |
| PHE66 | HD1 | 1.00 | 0.005 | 1.00 | 0.83 |
| PHE66 | HD2 | 1.00 | 0.005 | 1.00 | 0.83 |
| PHE66 | HE2 | 1.00 | 0.011 | 1.00 | 0.09 |
| PHE66 | H | 1.00 | 0.012 | 1.00 | -718077.00 |
| PHE66 | HE1 | 0.90 | 0.011 | 1.00 | 0.09 |
| GLY67 | H | 1.00 | 0.003 | 1.00 | -411723.00 |
| GLY67 | HA2 | 0.68 | 0.013 | 1.00 | 0.09 |

3.66.11 Detailed Probabilities of PHE66HB3:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE66 | 0.86 | 1.00 |
| GLY67 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F66HA | 1.00 |
| F66HB2 | 1.00 |
| F66HD1 | 1.00 |
| F66HD2 | 1.00 |
| F66HE2 | 1.00 |
| F66H | 1.00 |
| F66HB3 | 1.00 |
| G67H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE66 | HA | 1.00 | 0.007 | 1.00 | 0.22 |
| PHE66 | HB2 | 1.00 | 0.006 | 1.00 | 0.92 |
| PHE66 | HB3 | 1.00 | 0.007 | 1.00 | 0.87 |
| PHE66 | HD1 | 1.00 | 0.004 | 1.00 | 0.17 |
| PHE66 | HD2 | 1.00 | 0.004 | 1.00 | 0.17 |
| PHE66 | HE2 | 1.00 | 0.108 | 0.00 | 0.00 |
| PHE66 | H | 1.00 | 0.007 | 1.00 | -725670.00 |
| GLY67 | H | 1.00 | 0.013 | 1.00 | -252173.00 |

3.66.12 Detailed Probabilities of PHE66HD1:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE66 | 0.89 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F66HA | 1.00 |
| F66HB2 | 1.00 |
| F66HB3 | 1.00 |
| F66HD2 | 1.00 |
| F66HE1 | 1.00 |
| F66HE2 | 1.00 |
| F66HZ | 1.00 |
| F66H | 1.00 |
| F66HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE66 | HA | 1.00 | 0.004 | 1.00 | 0.66 |
| PHE66 | HB2 | 1.00 | 1.218 | 0.00 | 0.00 |
| PHE66 | HB3 | 1.00 | 0.004 | 1.00 | 0.18 |
| PHE66 | HD1 | 1.00 | 0.004 | 1.00 | 27.71 |
| PHE66 | HD2 | 1.00 | 0.004 | 1.00 | 27.71 |
| PHE66 | HE1 | 1.00 | 0.001 | 1.00 | 8.45 |
| PHE66 | HE2 | 1.00 | 0.001 | 1.00 | 8.45 |
| PHE66 | HZ | 1.00 | 0.004 | 1.00 | 0.10 |
| PHE66 | H | 1.00 | 0.005 | 1.00 | -280148.00 |

3.66.13 Detailed Probabilities of PHE66HD2:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE66 | 0.89 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F66HA | 1.00 |
| F66HB2 | 1.00 |
| F66HB3 | 1.00 |
| F66HD1 | 1.00 |
| F66HE1 | 1.00 |
| F66HE2 | 1.00 |
| F66HZ | 1.00 |
| F66H | 0.99 |
| F66HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE66 | HA | 1.00 | 0.004 | 1.00 | 0.66 |
| PHE66 | HB2 | 1.00 | 1.218 | 0.00 | 0.00 |
| PHE66 | HB3 | 1.00 | 0.004 | 1.00 | 0.18 |
| PHE66 | HD1 | 1.00 | 0.004 | 1.00 | 27.71 |
| PHE66 | HD2 | 1.00 | 0.004 | 1.00 | 27.71 |
| PHE66 | HE1 | 1.00 | 0.001 | 1.00 | 8.45 |
| PHE66 | HE2 | 1.00 | 0.001 | 1.00 | 8.45 |
| PHE66 | HZ | 1.00 | 0.004 | 1.00 | 0.10 |
| PHE66 | H | 0.99 | 0.005 | 1.00 | -280148.00 |

3.66.14 Detailed Probabilities of PHE66HE1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE66 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F66HD1 | 1.00 |
| F66HD2 | 1.00 |
| F66HE2 | 1.00 |
| F66HZ | 1.00 |
| F66HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE66 | HD1 | 1.00 | 0.005 | 1.00 | 2.23 |
| PHE66 | HD2 | 1.00 | 0.005 | 1.00 | 2.23 |
| PHE66 | HE1 | 1.00 | 0.004 | 1.00 | 6.93 |
| PHE66 | HE2 | 1.00 | 0.004 | 1.00 | 6.93 |
| PHE66 | HZ | 1.00 | 0.001 | 1.00 | 1.66 |
| PHE66 | HA | 0.74 | 0.006 | 1.00 | 0.14 |

3.66.15 Detailed Probabilities of PHE66HE2:

Overall probability: 0.715

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE66 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F66HB2 | 1.00 |
| F66HB3 | 1.00 |
| F66HD1 | 1.00 |
| F66HD2 | 1.00 |
| F66HE1 | 1.00 |
| F66HZ | 1.00 |
| F66HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE66 | HB2 | 1.00 | 1.413 | 0.00 | 0.00 |
| PHE66 | HB3 | 1.00 | 0.199 | 0.00 | 0.00 |
| PHE66 | HD1 | 1.00 | 0.005 | 1.00 | 2.23 |
| PHE66 | HD2 | 1.00 | 0.005 | 1.00 | 2.23 |
| PHE66 | HE1 | 1.00 | 0.004 | 1.00 | 6.93 |
| PHE66 | HE2 | 1.00 | 0.004 | 1.00 | 6.93 |
| PHE66 | HZ | 1.00 | 0.001 | 1.00 | 1.66 |

3.66.16 Detailed Probabilities of PHE66HZ:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE66 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F66HD1 | 1.00 |
| F66HD2 | 1.00 |
| F66HE1 | 1.00 |
| F66HE2 | 1.00 |
| F66HZ | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE66 | HD1 | 1.00 | 0.010 | 1.00 | 0.60 |
| PHE66 | HD2 | 1.00 | 0.010 | 1.00 | 0.60 |
| PHE66 | HE1 | 1.00 | 0.002 | 1.00 | 2.37 |
| PHE66 | HE2 | 1.00 | 0.002 | 1.00 | 2.37 |
| PHE66 | HZ | 1.00 | 0.002 | 1.00 | 2.55 |

3.66.17 Detailed Probabilities of PHE66H:

Overall probability: 0.929

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE65 | 0.83 | 1.00 |
| PHE66 | 1.00 | 1.00 |
| GLY67 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F65HB3 | 1.00 |
| F65HB2 | 1.00 |
| F65HA | 1.00 |
| F65H | 1.00 |
| F66HA | 1.00 |
| F66HB2 | 1.00 |
| F66HB3 | 1.00 |
| F66HD1 | 1.00 |
| F66HD2 | 0.99 |
| F66H | 1.00 |
| G67H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE65 | HA | 1.00 | 0.005 | 1.00 | 0.80 |
| PHE65 | HB2 | 1.00 | 0.006 | 1.00 | 0.12 |
| PHE65 | HB3 | 1.00 | 0.129 | 0.00 | 0.00 |
| PHE65 | H | 1.00 | 0.005 | 1.00 | -170848.00 |
| PHE65 | HD1 | 0.79 | 0.001 | 1.00 | 0.15 |
| PHE65 | HD2 | 0.70 | 0.001 | 1.00 | 0.15 |
| PHE66 | HA | 1.00 | 0.016 | 1.00 | 0.14 |
| PHE66 | HB2 | 1.00 | 0.006 | 1.00 | 0.17 |
| PHE66 | HB3 | 1.00 | 0.004 | 1.00 | 0.17 |
| PHE66 | HD1 | 1.00 | 0.001 | 1.00 | 0.18 |
| PHE66 | HD2 | 0.99 | 0.001 | 1.00 | 0.18 |
| PHE66 | H | 1.00 | 0.006 | 1.00 | -6412614.00 |
| GLY67 | H | 1.00 | 0.009 | 1.00 | -134253.00 |
| GLY67 | HA3 | 0.78 | 0.014 | 1.00 | 0.25 |

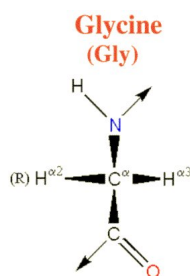
3.67 GLY(67)

Figure 57: Image from the BMRB

Residue probability: 0.802

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | NA | – | – | 0.000 | 0.000 |
| CA 3.67.1 | 43.016 | 45.581 | 4.381 | 0.800 | 1.000 |
| N 3.67.2 | 109.194 | 109.752 | 5.331 | 0.910 | 1.000 |
| HA2 3.67.3 | 3.886 | 3.967 | 0.380 | 0.429 | 1.000 |
| HA3 3.67.4 | 4.742 | 3.897 | 0.390 | 0.872 | 1.000 |
| H 3.67.5 | 8.558 | 8.343 | 0.939 | 1.000 | 1.000 |

3.67.1 Detailed Probabilities of GLY67CA:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE66 | 1.00 | 1.00 |
| GLY67 | 1.00 | 1.00 |
| PRO68 | 0.60 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F66HA | 1.00 |
| G67HA3 | 1.00 |
| G67H | 1.00 |
| G67HA2 | 1.00 |
| P68HD2 | 1.00 |
| P68HA | 1.00 |
| P68HD3 | 1.00 |

NOESY contacts detailed probability

3.67 GLY(67)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE66 | HA | 1.00 | 0.019 | 1.00 | 0.08 |
| PHE66 | HB2 | 0.68 | 0.013 | 1.00 | 0.09 |
| GLY67 | HA2 | 1.00 | 0.004 | 1.00 | 1.56 |
| GLY67 | HA3 | 1.00 | 0.003 | 1.00 | 1.43 |
| GLY67 | H | 1.00 | 0.002 | 1.00 | 0.39 |
| PRO68 | HA | 1.00 | 0.201 | 0.00 | 0.00 |
| PRO68 | HD2 | 1.00 | 0.003 | 1.00 | 0.50 |
| PRO68 | HD3 | 1.00 | 0.055 | 0.00 | 0.00 |
| PRO68 | HG2 | 0.84 | 0.004 | 1.00 | 0.07 |
| PRO68 | HG3 | 0.85 | 0.004 | 1.00 | 0.12 |

3.67.2 Detailed Probabilities of GLY67N:

Overall probability: 0.910

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE66 | 1.00 | 1.00 |
| GLY67 | 1.00 | 1.00 |
| PRO68 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F66HB2 | 1.00 |
| F66HB3 | 1.00 |
| F66HA | 1.00 |
| F66H | 1.00 |
| G67HA2 | 1.00 |
| G67HA3 | 1.00 |
| G67H | 1.00 |
| P68HD2 | 0.99 |
| P68HD3 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE66 | HA | 1.00 | 0.001 | 1.00 | -2343828.00 |
| PHE66 | HB2 | 1.00 | 0.003 | 1.00 | -411723.00 |
| PHE66 | HB3 | 1.00 | 0.013 | 1.00 | -252173.00 |
| PHE66 | H | 1.00 | 0.009 | 1.00 | -134253.00 |
| PHE66 | HD1 | 0.77 | 0.009 | 1.00 | -435397.00 |
| PHE66 | HD2 | 0.63 | 0.009 | 1.00 | -435397.00 |
| GLY67 | HA2 | 1.00 | 0.000 | 1.00 | -859025.00 |
| GLY67 | HA3 | 1.00 | 0.004 | 1.00 | -614800.00 |
| GLY67 | H | 1.00 | 0.005 | 1.00 | -7621914.00 |
| PRO68 | HD2 | 0.99 | 0.004 | 1.00 | -152395.00 |
| PRO68 | HD3 | 0.99 | 0.059 | 0.01 | 0.00 |

3.67.3 Detailed Probabilities of GLY67HA2:

Overall probability: 0.429

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE66 | 0.00 | 1.00 |
| GLY67 | 1.00 | 1.00 |
| PRO68 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F66HA | 1.00 |
| G67HA3 | 1.00 |
| G67H | 1.00 |
| G67HA2 | 1.00 |
| P68HD2 | 1.00 |
| P68HA | 1.00 |
| P68HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE66 | HA | 1.00 | 0.557 | 0.00 | 0.00 |
| GLY67 | HA2 | 1.00 | 0.004 | 1.00 | 1.56 |
| GLY67 | HA3 | 1.00 | 0.021 | 1.00 | 0.98 |
| GLY67 | H | 1.00 | 0.000 | 1.00 | -859025.00 |
| PRO68 | HA | 1.00 | 0.123 | 0.00 | 0.00 |
| PRO68 | HD2 | 1.00 | 0.060 | 0.00 | 0.00 |
| PRO68 | HD3 | 1.00 | 0.390 | 0.00 | 0.00 |

3.67.4 Detailed Probabilities of GLY67HA3:

Overall probability: 0.872

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE66 | 1.00 | 1.00 |
| GLY67 | 1.00 | 1.00 |
| PRO68 | 0.77 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F66HA | 1.00 |
| G67HA2 | 1.00 |
| G67H | 1.00 |
| G67HA3 | 1.00 |
| P68HD3 | 1.00 |
| P68HA | 1.00 |
| P68HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE66 | HA | 1.00 | 0.015 | 1.00 | 0.09 |
| GLY67 | HA2 | 1.00 | 0.003 | 1.00 | 1.43 |
| GLY67 | HA3 | 1.00 | 0.000 | 1.00 | 0.64 |
| GLY67 | H | 1.00 | 0.004 | 1.00 | -614800.00 |
| PRO68 | HA | 1.00 | 0.098 | 0.00 | 0.00 |
| PRO68 | HD2 | 1.00 | 0.004 | 1.00 | 0.58 |
| PRO68 | HD3 | 1.00 | 0.003 | 1.00 | 0.54 |
| PRO68 | HG2 | 0.85 | 0.034 | 0.85 | 0.00 |
| PRO68 | HG3 | 0.79 | 0.021 | 1.00 | 0.06 |

3.67.5 Detailed Probabilities of GLY67H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE66 | 1.00 | 1.00 |
| GLY67 | 1.00 | 1.00 |
| PRO68 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F66HB2 | 1.00 |
| F66HB3 | 1.00 |
| F66HA | 1.00 |
| F66H | 1.00 |
| G67HA2 | 1.00 |
| G67HA3 | 1.00 |
| G67H | 1.00 |
| P68HD2 | 0.99 |
| P68HD3 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE66 | HA | 1.00 | 0.006 | 1.00 | 0.79 |
| PHE66 | HB2 | 1.00 | 0.001 | 1.00 | 0.08 |
| PHE66 | HB3 | 1.00 | 0.010 | 1.00 | 0.08 |
| PHE66 | H | 1.00 | 0.004 | 1.00 | -104371.00 |
| PHE66 | HD1 | 0.77 | 0.012 | 1.00 | 0.08 |
| PHE66 | HD2 | 0.63 | 0.012 | 1.00 | 0.08 |
| GLY67 | HA2 | 1.00 | 0.002 | 1.00 | 0.39 |
| GLY67 | HA3 | 1.00 | 0.022 | 1.00 | 0.30 |
| GLY67 | H | 1.00 | 0.005 | 1.00 | -7621914.00 |
| PRO68 | HD2 | 0.99 | 0.013 | 1.00 | 0.07 |
| PRO68 | HD3 | 0.99 | 0.003 | 1.00 | 0.09 |

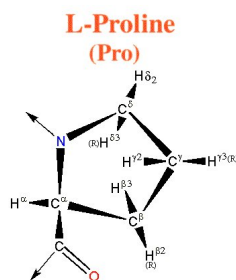
3.68 PRO(68)

Figure 58: Image from the BMRB

Residue probability: 0.679

Residue probability confidence: 0.951

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | NA | – | – | 0.000 | 0.000 |
| CA 3.68.1 | 64.167 | 62.931 | 15.301 | 0.600 | 0.909 |
| CB 3.68.2 | 31.942 | 33.632 | 13.629 | 0.600 | 0.875 |
| CG 3.68.3 | 27.601 | 28.412 | 13.801 | 0.857 | 1.000 |
| CD 3.68.4 | 49.045 | 49.797 | 3.175 | 0.900 | 1.000 |
| N | NA | – | – | 0.000 | 0.000 |
| HA 3.68.5 | 4.463 | 4.332 | 0.427 | 0.430 | 0.909 |
| HB2 3.68.6 | 1.875 | 2.099 | 0.501 | 0.778 | 0.889 |
| HB3 3.68.7 | 2.314 | 2.052 | 0.596 | 0.857 | 0.875 |
| HG2 3.68.8 | 2.084 | 1.927 | 0.364 | 0.714 | 1.000 |
| HG3 3.68.9 | 1.888 | 1.907 | 0.417 | 0.714 | 1.000 |
| HD2 3.68.10 | 3.500 | 3.640 | 0.682 | 0.700 | 1.000 |
| HD3 3.68.11 | 3.827 | 3.558 | 0.522 | 0.321 | 1.000 |

3.68.1 Detailed Probabilities of PRO68CA:

Overall probability: 0.600

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLY67 | 0.00 | 1.00 |
| PRO68 | 0.86 | 1.00 |
| ASP69 | 0.00 | 0.50 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| G67HA3 | 1.00 |
| G67HA2 | 1.00 |
| P68HB2 | 1.00 |
| P68HB3 | 1.00 |
| P68HG2 | 1.00 |
| P68HG3 | 1.00 |
| P68HD2 | 1.00 |
| P68HD3 | 1.00 |
| P68HA | 1.00 |
| D69H | 1.00 |
| D69HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLY67 | HA2 | 1.00 | 0.123 | 0.00 | 0.00 |
| GLY67 | HA3 | 1.00 | 0.098 | 0.00 | 0.00 |
| PRO68 | HA | 1.00 | 0.009 | 1.00 | 5.42 |
| PRO68 | HB2 | 1.00 | 0.007 | 1.00 | 0.75 |
| PRO68 | HB3 | 1.00 | 0.000 | 1.00 | 1.31 |
| PRO68 | HG2 | 1.00 | 0.017 | 1.00 | 0.26 |
| PRO68 | HG3 | 1.00 | 0.006 | 1.00 | 0.75 |
| PRO68 | HD2 | 1.00 | 0.003 | 1.00 | 0.17 |
| PRO68 | HD3 | 1.00 | 0.064 | 0.00 | 0.00 |
| ASP69 | HA | 1.00 | 0.136 | 0.00 | 0.00 |

3.68.2 Detailed Probabilities of PRO68CB:

Overall probability: 0.600

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO68 | 0.60 | 1.00 |
| ASP69 | 0.00 | 0.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P68HA | 1.00 |
| P68HB2 | 1.00 |
| P68HG2 | 1.00 |
| P68HG3 | 1.00 |
| P68HD2 | 1.00 |
| P68HD3 | 1.00 |
| P68HB3 | 1.00 |
| D69H | 1.00 |

NOESY contacts detailed probability

3.68 PRO(68)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO68 | HA | 1.00 | 0.043 | 0.00 | 0.00 |
| PRO68 | HB2 | 1.00 | 0.005 | 1.00 | 6.76 |
| PRO68 | HB3 | 1.00 | 0.002 | 1.00 | 21.15 |
| PRO68 | HG2 | 1.00 | 0.020 | 1.00 | 2.26 |
| PRO68 | HG3 | 1.00 | 0.008 | 1.00 | 6.76 |
| PRO68 | HD2 | 1.00 | 0.072 | 0.00 | 0.00 |
| PRO68 | HD3 | 1.00 | 0.038 | 0.20 | 0.00 |

3.68.3 Detailed Probabilities of PRO68CG:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO68 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P68HA | 1.00 |
| P68HB2 | 1.00 |
| P68HB3 | 1.00 |
| P68HG2 | 1.00 |
| P68HD2 | 1.00 |
| P68HD3 | 1.00 |
| P68HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO68 | HA | 1.00 | 0.045 | 0.00 | 0.00 |
| PRO68 | HB2 | 1.00 | 0.014 | 1.00 | 9.37 |
| PRO68 | HB3 | 1.00 | 0.002 | 1.00 | 1.15 |
| PRO68 | HG2 | 1.00 | 0.018 | 1.00 | 4.46 |
| PRO68 | HG3 | 1.00 | 0.001 | 1.00 | 9.37 |
| PRO68 | HD2 | 1.00 | 0.002 | 1.00 | 0.68 |
| PRO68 | HD3 | 1.00 | 0.005 | 1.00 | 0.90 |

3.68.4 Detailed Probabilities of PRO68CD:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLY67 | 0.67 | 1.00 |
| PRO68 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| G67HA3 | 1.00 |
| G67H | 0.99 |
| G67HA2 | 1.00 |
| P68HA | 1.00 |
| P68HB2 | 1.00 |
| P68HB3 | 1.00 |
| P68HG2 | 1.00 |
| P68HG3 | 1.00 |
| P68HD3 | 1.00 |
| P68HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLY67 | HA2 | 1.00 | 0.060 | 0.00 | 0.00 |
| GLY67 | HA3 | 1.00 | 0.004 | 1.00 | 0.58 |
| GLY67 | H | 0.99 | 0.013 | 1.00 | 0.07 |
| PRO68 | HA | 1.00 | 0.012 | 1.00 | 0.10 |
| PRO68 | HB2 | 1.00 | 0.014 | 1.00 | 0.79 |
| PRO68 | HB3 | 1.00 | 0.004 | 1.00 | 0.21 |
| PRO68 | HG2 | 1.00 | 0.003 | 1.00 | 0.56 |
| PRO68 | HG3 | 1.00 | 0.001 | 1.00 | 0.79 |
| PRO68 | HD2 | 1.00 | 0.003 | 1.00 | 3.20 |
| PRO68 | HD3 | 1.00 | 0.001 | 1.00 | 2.71 |

3.68.5 Detailed Probabilities of PRO68HA:

Overall probability: 0.430

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLY67 | 0.00 | 1.00 |
| PRO68 | 0.61 | 1.00 |
| ASP69 | 0.00 | 0.50 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| G67HA3 | 1.00 |
| G67HA2 | 1.00 |
| P68HB2 | 1.00 |
| P68HB3 | 1.00 |
| P68HG2 | 1.00 |
| P68HG3 | 1.00 |
| P68HD2 | 1.00 |
| P68HD3 | 1.00 |
| P68HA | 1.00 |
| D69H | 1.00 |
| D69HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLY67 | HA2 | 1.00 | 0.201 | 0.00 | 0.00 |
| GLY67 | HA3 | 1.00 | 0.041 | 0.00 | 0.00 |
| PRO68 | HA | 1.00 | 0.009 | 1.00 | 5.42 |
| PRO68 | HB2 | 1.00 | 0.037 | 0.30 | 0.00 |
| PRO68 | HB3 | 1.00 | 0.043 | 0.00 | 0.00 |
| PRO68 | HG2 | 1.00 | 0.013 | 1.00 | 0.48 |
| PRO68 | HG3 | 1.00 | 0.045 | 0.00 | 0.00 |
| PRO68 | HD2 | 1.00 | 0.012 | 1.00 | 0.10 |
| PRO68 | HD3 | 1.00 | 0.010 | 1.00 | 0.10 |
| ASP69 | HA | 1.00 | 0.048 | 0.00 | 0.00 |

3.68.6 Detailed Probabilities of PRO68HB2:

Overall probability: 0.778

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO68 | 0.71 | 1.00 |
| ASP69 | 1.00 | 0.50 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P68HA | 1.00 |
| P68HB3 | 1.00 |
| P68HG2 | 1.00 |
| P68HG3 | 1.00 |
| P68HD2 | 1.00 |
| P68HD3 | 1.00 |
| P68HB2 | 1.00 |
| D69HA | 0.99 |
| D69H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO68 | HA | 1.00 | 0.007 | 1.00 | 0.75 |
| PRO68 | HB2 | 1.00 | 0.444 | 0.00 | 0.00 |
| PRO68 | HB3 | 1.00 | 0.005 | 1.00 | 6.76 |
| PRO68 | HG2 | 1.00 | 0.016 | 1.00 | 5.40 |
| PRO68 | HG3 | 1.00 | 0.014 | 1.00 | 9.37 |
| PRO68 | HD2 | 1.00 | 0.014 | 1.00 | 0.79 |
| PRO68 | HD3 | 1.00 | 0.544 | 0.00 | 0.00 |
| ASP69 | HA | 0.99 | 0.023 | 1.00 | 0.24 |
| ASP69 | HB2 | 0.64 | 0.004 | 1.00 | 0.06 |

3.68.7 Detailed Probabilities of PRO68HB3:

Overall probability: 0.857

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO68 | 0.86 | 1.00 |
| ASP69 | 0.00 | 0.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P68HA | 1.00 |
| P68HB2 | 1.00 |
| P68HG2 | 1.00 |
| P68HG3 | 1.00 |
| P68HD2 | 1.00 |
| P68HD3 | 1.00 |
| P68HB3 | 1.00 |
| D69H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO68 | HA | 1.00 | 0.000 | 1.00 | 1.31 |
| PRO68 | HB2 | 1.00 | 0.012 | 1.00 | 6.08 |
| PRO68 | HB3 | 1.00 | 0.002 | 1.00 | 21.15 |
| PRO68 | HG2 | 1.00 | 0.013 | 1.00 | 3.73 |
| PRO68 | HG3 | 1.00 | 0.002 | 1.00 | 1.15 |
| PRO68 | HD2 | 1.00 | 0.004 | 1.00 | 0.21 |
| PRO68 | HD3 | 1.00 | 0.983 | 0.00 | 0.00 |

3.68.8 Detailed Probabilities of PRO68HG2:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO68 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P68HA | 1.00 |
| P68HB2 | 1.00 |
| P68HB3 | 1.00 |
| P68HG3 | 1.00 |
| P68HD2 | 1.00 |
| P68HD3 | 1.00 |
| P68HG2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO68 | HA | 1.00 | 0.017 | 1.00 | 0.26 |
| PRO68 | HB2 | 1.00 | 0.242 | 0.00 | 0.00 |
| PRO68 | HB3 | 1.00 | 0.020 | 1.00 | 2.26 |
| PRO68 | HG2 | 1.00 | 0.001 | 1.00 | 31.34 |
| PRO68 | HG3 | 1.00 | 0.018 | 1.00 | 4.46 |
| PRO68 | HD2 | 1.00 | 0.003 | 1.00 | 0.56 |
| PRO68 | HD3 | 1.00 | 0.753 | 0.00 | 0.00 |

3.68.9 Detailed Probabilities of PRO68HG3:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO68 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P68HA | 1.00 |
| P68HB2 | 1.00 |
| P68HB3 | 1.00 |
| P68HG2 | 1.00 |
| P68HD2 | 1.00 |
| P68HD3 | 1.00 |
| P68HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO68 | HA | 1.00 | 0.006 | 1.00 | 0.75 |
| PRO68 | HB2 | 1.00 | 0.438 | 0.00 | 0.00 |
| PRO68 | HB3 | 1.00 | 0.008 | 1.00 | 6.76 |
| PRO68 | HG2 | 1.00 | 0.003 | 1.00 | 5.40 |
| PRO68 | HG3 | 1.00 | 0.001 | 1.00 | 9.37 |
| PRO68 | HD2 | 1.00 | 0.001 | 1.00 | 0.79 |
| PRO68 | HD3 | 1.00 | 0.557 | 0.00 | 0.00 |

3.68.10 Detailed Probabilities of PRO68HD2:

Overall probability: 0.700

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLY67 | 0.67 | 1.00 |
| PRO68 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| G67HA3 | 1.00 |
| G67H | 0.99 |
| G67HA2 | 1.00 |
| P68HA | 1.00 |
| P68HB2 | 1.00 |
| P68HB3 | 1.00 |
| P68HG2 | 1.00 |
| P68HG3 | 1.00 |
| P68HD3 | 1.00 |
| P68HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLY67 | HA2 | 1.00 | 0.003 | 1.00 | 0.50 |
| GLY67 | HA3 | 1.00 | 0.116 | 0.00 | 0.00 |
| GLY67 | H | 0.99 | 0.004 | 1.00 | -152395.00 |
| PRO68 | HA | 1.00 | 0.003 | 1.00 | 0.17 |
| PRO68 | HB2 | 1.00 | 0.330 | 0.00 | 0.00 |
| PRO68 | HB3 | 1.00 | 0.072 | 0.00 | 0.00 |
| PRO68 | HG2 | 1.00 | 0.013 | 1.00 | 0.65 |
| PRO68 | HG3 | 1.00 | 0.002 | 1.00 | 0.68 |
| PRO68 | HD2 | 1.00 | 0.003 | 1.00 | 3.20 |
| PRO68 | HD3 | 1.00 | 0.004 | 1.00 | 2.74 |

3.68.11 Detailed Probabilities of PRO68HD3:

Overall probability: 0.321

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLY67 | 0.34 | 1.00 |
| PRO68 | 0.31 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| G67H | 0.99 |
| G67HA2 | 1.00 |
| G67HA3 | 1.00 |
| P68HA | 1.00 |
| P68HB2 | 1.00 |
| P68HB3 | 1.00 |
| P68HG2 | 1.00 |
| P68HG3 | 1.00 |
| P68HD2 | 1.00 |
| P68HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLY67 | HA2 | 1.00 | 0.055 | 0.00 | 0.00 |
| GLY67 | HA3 | 1.00 | 0.002 | 1.00 | 0.53 |
| GLY67 | H | 0.99 | 0.059 | 0.01 | 0.00 |
| PRO68 | HA | 1.00 | 0.064 | 0.00 | 0.00 |
| PRO68 | HB2 | 1.00 | 0.216 | 0.00 | 0.00 |
| PRO68 | HB3 | 1.00 | 0.038 | 0.20 | 0.00 |
| PRO68 | HG2 | 1.00 | 0.057 | 0.00 | 0.00 |
| PRO68 | HG3 | 1.00 | 0.005 | 1.00 | 0.90 |
| PRO68 | HD2 | 1.00 | 0.001 | 1.00 | 2.71 |
| PRO68 | HD3 | 1.00 | 0.331 | 0.00 | 0.00 |

3.69 ASP(69)

Figure 59: Image from the BMRB

Residue probability: 0.697

Residue probability confidence: 0.711

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 174.508 | 176.463 | 2.348 | 0.000 | 0.000 |
| CA 3.69.1 | 52.258 | 54.786 | 4.266 | 0.543 | 0.778 |
| CB 3.69.2 | 41.452 | 40.949 | 3.070 | 1.000 | 0.667 |
| N | NA | – | – | 0.000 | 0.000 |
| HD2 | NA | – | – | 0.000 | 0.000 |
| HA 3.69.3 | 4.704 | 4.587 | 0.329 | 0.430 | 0.778 |
| HB2 3.69.4 | 2.924 | 2.708 | 0.282 | 0.750 | 0.667 |
| HB3 3.69.5 | 2.606 | 2.654 | 0.285 | 0.760 | 0.667 |
| H | NA | – | – | 0.000 | 0.000 |

3.69.1 Detailed Probabilities of ASP69CA:

Overall probability: 0.543

Overall confidence: 0.778

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO68 | 0.50 | 1.00 |
| ASP69 | 0.93 | 0.60 |
| SER70 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P68HA | 1.00 |
| P68HB2 | 0.99 |
| D69HD2 | 1.00 |
| D69HB2 | 1.00 |
| D69HB3 | 1.00 |
| D69H | 1.00 |
| D69HA | 1.00 |
| S70H | 1.00 |
| S70HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO68 | HA | 1.00 | 0.048 | 0.00 | 0.00 |
| PRO68 | HB2 | 0.99 | 0.023 | 1.00 | 0.24 |
| ASP69 | HA | 1.00 | 0.024 | 1.00 | 9.08 |
| ASP69 | HB2 | 1.00 | 0.010 | 1.00 | 1.27 |
| ASP69 | HB3 | 1.00 | 0.032 | 0.80 | 0.00 |
| SER70 | HA | 1.00 | 0.138 | 0.00 | 0.00 |
| SER70 | H | 1.00 | 0.106 | 0.00 | 0.00 |

3.69.2 Detailed Probabilities of ASP69CB:

Overall probability: 1.000

Overall confidence: 0.667

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP69 | 1.00 | 0.60 |
| SER70 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D69HD2 | 1.00 |
| D69HA | 1.00 |
| D69HB2 | 1.00 |
| D69H | 1.00 |
| D69HB3 | 1.00 |
| S70H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP69 | HA | 1.00 | 0.003 | 1.00 | 0.68 |
| ASP69 | HB2 | 1.00 | 0.009 | 1.00 | 3.52 |
| ASP69 | HB3 | 1.00 | 0.004 | 1.00 | 4.06 |
| SER70 | H | 1.00 | 0.003 | 1.00 | 0.05 |

3.69.3 Detailed Probabilities of ASP69HA:

Overall probability: 0.430

Overall confidence: 0.778

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO68 | 0.01 | 1.00 |
| ASP69 | 0.67 | 0.60 |
| SER70 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P68HA | 1.00 |
| P68HB2 | 0.99 |
| D69HD2 | 1.00 |
| D69HB2 | 1.00 |
| D69HB3 | 1.00 |
| D69H | 1.00 |
| D69HA | 1.00 |
| S70H | 1.00 |
| S70HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO68 | HA | 1.00 | 0.136 | 0.00 | 0.00 |
| PRO68 | HB2 | 0.99 | 0.204 | 0.01 | 0.00 |
| ASP69 | HA | 1.00 | 0.024 | 1.00 | 9.08 |
| ASP69 | HB2 | 1.00 | 0.369 | 0.00 | 0.00 |
| ASP69 | HB3 | 1.00 | 0.003 | 1.00 | 0.68 |
| SER70 | HA | 1.00 | 0.006 | 1.00 | 0.55 |
| SER70 | H | 1.00 | 0.096 | 0.00 | 0.00 |

3.69.4 Detailed Probabilities of ASP69HB2:

Overall probability: 0.750

Overall confidence: 0.667

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP69 | 0.67 | 0.60 |
| SER70 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D69HD2 | 1.00 |
| D69HA | 1.00 |
| D69HB3 | 1.00 |
| D69H | 1.00 |
| D69HB2 | 1.00 |
| S70H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP69 | HA | 1.00 | 0.010 | 1.00 | 1.27 |
| ASP69 | HB2 | 1.00 | 0.603 | 0.00 | 0.00 |
| ASP69 | HB3 | 1.00 | 0.009 | 1.00 | 3.52 |
| SER70 | H | 1.00 | 0.013 | 1.00 | -91470.00 |

3.69.5 Detailed Probabilities of ASP69HB3:

Overall probability: 0.760

Overall confidence: 0.667

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP69 | 0.60 | 0.60 |
| SER70 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D69HD2 | 1.00 |
| D69HA | 1.00 |
| D69HB2 | 1.00 |
| D69H | 1.00 |
| D69HB3 | 1.00 |
| S70H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP69 | HA | 1.00 | 0.032 | 0.80 | 0.00 |
| ASP69 | HB2 | 1.00 | 0.285 | 0.00 | 0.00 |
| ASP69 | HB3 | 1.00 | 0.004 | 1.00 | 4.06 |
| SER70 | H | 1.00 | 0.004 | 1.00 | -98884.00 |
| SER70 | HA | 0.82 | 0.016 | 1.00 | 0.17 |

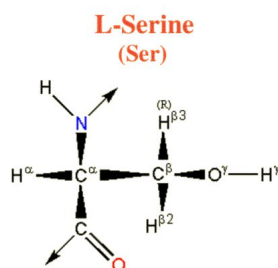
3.70 SER(70)

Figure 60: Image from the BMRB

Residue probability: 0.795

Residue probability confidence: 0.836

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 171.414 | 174.682 | 1.868 | 0.000 | 0.000 |
| CA 3.70.1 | 57.424 | 58.750 | 3.025 | 1.000 | 0.875 |
| CB 3.70.2 | 66.693 | 63.523 | 4.288 | 0.800 | 0.833 |
| N 3.70.3 | 109.416 | 116.135 | 5.326 | 0.750 | 0.800 |
| HA 3.70.4 | 5.098 | 4.486 | 0.430 | 0.714 | 0.875 |
| HB2 3.70.5 | 3.614 | 3.856 | 0.325 | 0.800 | 0.833 |
| HB3 3.70.6 | 3.901 | 3.825 | 0.343 | 1.000 | 0.833 |
| H 3.70.7 | 7.226 | 8.292 | 0.600 | 0.500 | 0.800 |
| HG | NA | – | – | 0.000 | 0.000 |

3.70.1 Detailed Probabilities of SER70CA:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP69 | 1.00 | 1.00 |
| SER70 | 1.00 | 0.80 |
| ILE71 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D69HA | 1.00 |
| S70HB2 | 1.00 |
| S70HB3 | 1.00 |
| S70H | 1.00 |
| S70HG | 1.00 |
| S70HA | 1.00 |
| I71HA | 1.00 |
| I71H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP69 | HA | 1.00 | 0.006 | 1.00 | 0.55 |
| ASP69 | HB3 | 0.82 | 0.016 | 1.00 | 0.17 |
| SER70 | HA | 1.00 | 0.003 | 1.00 | 2.77 |
| SER70 | HB2 | 1.00 | 0.011 | 1.00 | 0.55 |
| SER70 | HB3 | 1.00 | 0.008 | 1.00 | 0.72 |
| SER70 | H | 1.00 | 0.017 | 1.00 | 0.11 |
| ILE71 | HA | 1.00 | 0.011 | 1.00 | 0.17 |
| ILE71 | H | 1.00 | 0.008 | 1.00 | 0.90 |
| ILE71 | HG13 | 0.62 | 0.029 | 1.00 | 0.31 |

3.70.2 Detailed Probabilities of SER70CB:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER70 | 0.75 | 0.80 |
| ILE71 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S70HA | 1.00 |
| S70HB3 | 1.00 |
| S70H | 1.00 |
| S70HG | 1.00 |
| S70HB2 | 1.00 |
| I71H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER70 | HA | 1.00 | 0.007 | 1.00 | 0.57 |
| SER70 | HB2 | 1.00 | 0.005 | 1.00 | 1.66 |
| SER70 | HB3 | 1.00 | 0.004 | 1.00 | 1.58 |
| SER70 | H | 1.00 | 1.972 | 0.00 | 0.00 |
| ILE71 | H | 1.00 | 0.007 | 1.00 | 0.45 |

3.70.3 Detailed Probabilities of SER70N:

Overall probability: 0.750

Overall confidence: 0.800

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP69 | 0.67 | 0.75 |
| SER70 | 0.75 | 0.80 |
| ILE71 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D69H | 1.00 |
| D69HB2 | 1.00 |
| D69HA | 1.00 |
| D69HB3 | 1.00 |
| S70HA | 1.00 |
| S70HB2 | 1.00 |
| S70HB3 | 1.00 |
| S70HG | 1.00 |
| S70H | 1.00 |
| I71H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP69 | HA | 1.00 | 0.096 | 0.00 | 0.00 |
| ASP69 | HB2 | 1.00 | 0.013 | 1.00 | -91470.00 |
| ASP69 | HB3 | 1.00 | 0.004 | 1.00 | -98884.00 |
| SER70 | HA | 1.00 | 0.007 | 1.00 | -764246.00 |
| SER70 | HB2 | 1.00 | 0.087 | 0.00 | 0.00 |
| SER70 | HB3 | 1.00 | 0.010 | 1.00 | -559546.00 |
| SER70 | H | 1.00 | 0.004 | 1.00 | -13554855.00 |
| ILE71 | H | 1.00 | 0.004 | 1.00 | -179463.00 |

3.70.4 Detailed Probabilities of SER70HA:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP69 | 0.00 | 1.00 |
| SER70 | 1.00 | 0.80 |
| ILE71 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D69HA | 1.00 |
| S70HB2 | 1.00 |
| S70HB3 | 1.00 |
| S70H | 1.00 |
| S70HG | 1.00 |
| S70HA | 1.00 |
| I71HA | 1.00 |
| I71H | 1.00 |

NOESY contacts detailed probability

3.70 SER(70)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP69 | HA | 1.00 | 0.138 | 0.00 | 0.00 |
| SER70 | HA | 1.00 | 0.003 | 1.00 | 2.77 |
| SER70 | HB2 | 1.00 | 0.007 | 1.00 | 0.57 |
| SER70 | HB3 | 1.00 | 0.005 | 1.00 | 0.60 |
| SER70 | H | 1.00 | 0.007 | 1.00 | -764246.00 |
| ILE71 | HA | 1.00 | 0.079 | 0.00 | 0.00 |
| ILE71 | H | 1.00 | 0.006 | 1.00 | -1365183.00 |

3.70.5 Detailed Probabilities of SER70HB2:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER70 | 0.75 | 0.80 |
| ILE71 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S70HA | 1.00 |
| S70HB3 | 1.00 |
| S70H | 1.00 |
| S70HG | 1.00 |
| S70HB2 | 1.00 |
| I71H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER70 | HA | 1.00 | 0.011 | 1.00 | 0.55 |
| SER70 | HB2 | 1.00 | 0.005 | 1.00 | 1.66 |
| SER70 | HB3 | 1.00 | 0.003 | 1.00 | 1.54 |
| SER70 | H | 1.00 | 0.087 | 0.00 | 0.00 |
| ILE71 | H | 1.00 | 0.003 | 1.00 | -761024.00 |

3.70.6 Detailed Probabilities of SER70HB3:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER70 | 1.00 | 0.80 |
| ILE71 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S70HA | 1.00 |
| S70HB2 | 1.00 |
| S70H | 1.00 |
| S70HG | 1.00 |
| S70HB3 | 1.00 |
| I71H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER70 | HA | 1.00 | 0.008 | 1.00 | 0.72 |
| SER70 | HB2 | 1.00 | 0.004 | 1.00 | 1.58 |
| SER70 | HB3 | 1.00 | 0.001 | 1.00 | 2.09 |
| SER70 | H | 1.00 | 0.010 | 1.00 | -559546.00 |
| ILE71 | H | 1.00 | 0.012 | 1.00 | -598325.00 |

3.70.7 Detailed Probabilities of SER70H:

Overall probability: 0.500

Overall confidence: 0.800

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP69 | 0.33 | 0.75 |
| SER70 | 0.50 | 0.80 |
| ILE71 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D69H | 1.00 |
| D69HB2 | 1.00 |
| D69HA | 1.00 |
| D69HB3 | 1.00 |
| S70HA | 1.00 |
| S70HB2 | 1.00 |
| S70HB3 | 1.00 |
| S70HG | 1.00 |
| S70H | 1.00 |
| I71H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP69 | HA | 1.00 | 0.106 | 0.00 | 0.00 |
| ASP69 | HB2 | 1.00 | 0.646 | 0.00 | 0.00 |
| ASP69 | HB3 | 1.00 | 0.003 | 1.00 | 0.05 |
| SER70 | HA | 1.00 | 0.017 | 1.00 | 0.11 |
| SER70 | HB2 | 1.00 | 1.972 | 0.00 | 0.00 |
| SER70 | HB3 | 1.00 | 1.973 | 0.00 | 0.00 |
| SER70 | H | 1.00 | 0.004 | 1.00 | -13554855.00 |
| ILE71 | H | 1.00 | 0.017 | 1.00 | -171442.00 |

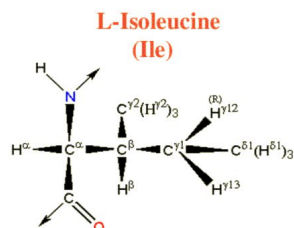


Figure 61: Image from the BMRB

Residue probability: 0.838
Residue probability confidence: 0.987

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|--------------|-------------|---------|--------|---------------------|--------------------|
| C | 175.366 | 175.926 | 2.710 | 0.000 | 0.000 |
| CA 3.71.1 | 60.460 | 61.717 | 4.152 | 0.780 | 1.000 |
| CB 3.71.2 | 42.854 | 38.702 | 3.945 | 0.912 | 1.000 |
| CG1 3.71.3 | 28.132 | 27.785 | 2.037 | 0.863 | 1.000 |
| CG2 3.71.4 | 17.663 | 17.574 | 1.928 | 0.700 | 1.000 |
| CD1 3.71.5 | 15.672 | 13.545 | 3.646 | 0.900 | 1.000 |
| N 3.71.6 | 120.092 | 121.467 | 6.098 | 0.967 | 0.917 |
| HA 3.71.7 | 5.168 | 4.185 | 1.403 | 0.900 | 1.000 |
| HB 3.71.8 | 1.761 | 1.776 | 0.310 | 0.750 | 1.000 |
| HG12 3.71.9 | 1.563 | 1.271 | 0.411 | 1.000 | 1.000 |
| HG13 3.71.10 | 0.979 | 1.186 | 0.426 | 0.429 | 1.000 |
| HG2 3.71.11 | 0.942 | 0.762 | 0.283 | 0.889 | 1.000 |
| HD1 3.71.12 | 0.703 | 0.668 | 0.293 | 0.886 | 1.000 |
| H 3.71.13 | 9.191 | 8.301 | 0.685 | 0.917 | 0.917 |

3.71.1 Detailed Probabilities of ILE71CA:

Overall probability: 0.780
Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|--------------|-------------|-------------|
| SER70 | 0.00 | 1.00 |
| ILE71 | 0.97 | 1.00 |
| THR72 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| S70HA | 1.00 |
| I71HB | 1.00 |
| I71HG12 | 1.00 |
| I71HG13 | 1.00 |
| I71HG21 | 1.00 |
| I71HD11 | 0.97 |
| I71H | 1.00 |
| I71HA | 1.00 |
| T72HA | 1.00 |
| T72H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER70 | HA | 1.00 | 0.079 | 0.00 | 0.00 |
| ILE71 | HA | 1.00 | 0.009 | 1.00 | 2.80 |
| ILE71 | HB | 1.00 | 0.001 | 1.00 | 0.24 |
| ILE71 | HG12 | 1.00 | 0.017 | 1.00 | 0.29 |
| ILE71 | HG13 | 1.00 | 0.032 | 0.80 | 0.00 |
| ILE71 | HG21 | 1.00 | 0.005 | 1.00 | 0.65 |
| ILE71 | HD11 | 0.97 | 0.008 | 1.00 | 0.34 |
| ILE71 | H | 1.00 | 0.023 | 1.00 | 0.22 |
| THR72 | HA | 1.00 | 0.101 | 0.00 | 0.00 |
| THR72 | H | 1.00 | 0.008 | 1.00 | 0.77 |

3.71.2 Detailed Probabilities of ILE71CB:

Overall probability: 0.912

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE71 | 0.90 | 1.00 |
| THR72 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I71HA | 1.00 |
| I71HG12 | 1.00 |
| I71HG13 | 1.00 |
| I71HG21 | 1.00 |
| I71HD11 | 1.00 |
| I71H | 1.00 |
| I71HB | 1.00 |
| T72H | 1.00 |

NOESY contacts detailed probability

3.71 ILE(71)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE71 | HA | 1.00 | 0.007 | 1.00 | 0.15 |
| ILE71 | HB | 1.00 | 0.001 | 1.00 | 2.87 |
| ILE71 | HG12 | 1.00 | 0.009 | 1.00 | 0.53 |
| ILE71 | HG13 | 1.00 | 0.037 | 0.30 | 0.00 |
| ILE71 | HG21 | 1.00 | 0.000 | 1.00 | 1.21 |
| ILE71 | HD11 | 1.00 | 0.004 | 1.00 | 0.83 |
| ILE71 | H | 1.00 | 0.007 | 1.00 | 0.38 |
| THR72 | H | 1.00 | 0.002 | 1.00 | 0.07 |

3.71.3 Detailed Probabilities of ILE71CG1:

Overall probability: 0.863

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE71 | 0.84 | 1.00 |
| THR72 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I71HA | 1.00 |
| I71HB | 1.00 |
| I71HG13 | 1.00 |
| I71HG21 | 1.00 |
| I71HD11 | 1.00 |
| I71H | 1.00 |
| I71HG12 | 1.00 |
| T72H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE71 | HA | 1.00 | 0.008 | 1.00 | 0.36 |
| ILE71 | HB | 1.00 | 0.007 | 1.00 | 0.56 |
| ILE71 | HG12 | 1.00 | 0.012 | 1.00 | 15.92 |
| ILE71 | HG13 | 1.00 | 0.011 | 1.00 | 2.78 |
| ILE71 | HG21 | 1.00 | 0.026 | 1.00 | 2.78 |
| ILE71 | HD11 | 1.00 | 0.031 | 0.90 | 0.00 |
| ILE71 | H | 1.00 | 0.831 | 0.00 | 0.00 |
| THR72 | H | 0.98 | 0.000 | 1.00 | 0.06 |

3.71.4 Detailed Probabilities of ILE71CG2:

Overall probability: 0.700

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE71 | 0.61 | 1.00 |
| THR72 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I71HA | 1.00 |
| I71HB | 1.00 |
| I71HG12 | 1.00 |
| I71HG13 | 1.00 |
| I71HG22 | 1.00 |
| I71HD11 | 0.99 |
| I71H | 1.00 |
| T72H | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE71 | HA | 1.00 | 0.009 | 1.00 | 0.53 |
| ILE71 | HB | 1.00 | 0.042 | 0.00 | 0.00 |
| ILE71 | HG12 | 1.00 | 0.004 | 1.00 | 0.45 |
| ILE71 | HG13 | 1.00 | 0.062 | 0.00 | 0.00 |
| ILE71 | HG21 | 1.00 | 0.025 | 1.00 | 72.70 |
| ILE71 | HD11 | 0.99 | 0.037 | 0.30 | 0.00 |
| ILE71 | H | 1.00 | 0.016 | 1.00 | 0.16 |
| THR72 | H | 0.99 | 0.006 | 1.00 | 0.31 |
| THR72 | HA | 0.64 | 0.002 | 1.00 | 0.08 |

3.71.5 Detailed Probabilities of ILE71CD1:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE71 | 0.90 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I71HA | 0.97 |
| I71HB | 1.00 |
| I71HG12 | 1.00 |
| I71HG13 | 1.00 |
| I71HG21 | 0.99 |
| I71HD12 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE71 | HA | 0.97 | 0.010 | 1.00 | 0.20 |
| ILE71 | HB | 1.00 | 0.003 | 1.00 | 1.25 |
| ILE71 | HG12 | 1.00 | 0.012 | 1.00 | 1.37 |
| ILE71 | HG13 | 1.00 | 0.037 | 0.30 | 0.00 |
| ILE71 | HG21 | 0.99 | 0.000 | 1.00 | 3.08 |
| ILE71 | HD11 | 1.00 | 0.003 | 1.00 | 51.50 |
| ILE71 | H | 0.94 | 0.010 | 1.00 | 0.26 |

3.71.6 Detailed Probabilities of ILE71N:

Overall probability: 0.967

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER70 | 1.00 | 0.80 |
| ILE71 | 0.94 | 1.00 |
| THR72 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| S70HA | 1.00 |
| S70HG | 0.98 |
| S70H | 1.00 |
| S70HB3 | 1.00 |
| S70HB2 | 1.00 |
| I71HA | 1.00 |
| I71HB | 1.00 |
| I71HG12 | 1.00 |
| I71HG13 | 1.00 |
| I71HG21 | 1.00 |
| I71H | 1.00 |
| T72H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER70 | HA | 1.00 | 0.006 | 1.00 | -1365183.00 |
| SER70 | HB2 | 1.00 | 0.003 | 1.00 | -761024.00 |
| SER70 | HB3 | 1.00 | 0.012 | 1.00 | -598325.00 |
| SER70 | H | 1.00 | 0.017 | 1.00 | -171442.00 |
| ILE71 | HA | 1.00 | 0.001 | 1.00 | -415722.00 |
| ILE71 | HB | 1.00 | 0.001 | 1.00 | -806568.00 |
| ILE71 | HG12 | 1.00 | 0.012 | 1.00 | -415117.00 |
| ILE71 | HG13 | 1.00 | 0.034 | 0.60 | 0.00 |
| ILE71 | HG21 | 1.00 | 0.003 | 1.00 | -575677.00 |
| ILE71 | H | 1.00 | 0.007 | 1.00 | -5820170.00 |
| ILE71 | HD11 | 0.94 | 0.014 | 1.00 | -634581.00 |
| THR72 | H | 1.00 | 0.002 | 1.00 | -110747.00 |

3.71.7 Detailed Probabilities of ILE71HA:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER70 | 1.00 | 1.00 |
| ILE71 | 1.00 | 1.00 |
| THR72 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| S70HA | 1.00 |
| I71HB | 1.00 |
| I71HG12 | 1.00 |
| I71HG13 | 1.00 |
| I71HG21 | 1.00 |
| I71HD11 | 0.97 |
| I71H | 1.00 |
| I71HA | 1.00 |
| T72HA | 1.00 |
| T72H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER70 | HA | 1.00 | 0.011 | 1.00 | 0.17 |
| ILE71 | HA | 1.00 | 0.009 | 1.00 | 2.80 |
| ILE71 | HB | 1.00 | 0.007 | 1.00 | 0.15 |
| ILE71 | HG12 | 1.00 | 0.008 | 1.00 | 0.36 |
| ILE71 | HG13 | 1.00 | 0.009 | 1.00 | 0.35 |
| ILE71 | HG21 | 1.00 | 0.009 | 1.00 | 0.53 |
| ILE71 | HD11 | 0.97 | 0.010 | 1.00 | 0.20 |
| ILE71 | H | 1.00 | 0.001 | 1.00 | -415722.00 |
| THR72 | HA | 1.00 | 0.330 | 0.00 | 0.00 |
| THR72 | H | 1.00 | 0.008 | 1.00 | -1572376.00 |

3.71.8 Detailed Probabilities of ILE71HB:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE71 | 0.71 | 1.00 |
| THR72 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I71HA | 1.00 |
| I71HG12 | 1.00 |
| I71HG13 | 1.00 |
| I71HG21 | 1.00 |
| I71HD11 | 1.00 |
| I71H | 1.00 |
| I71HB | 1.00 |
| T72H | 1.00 |

NOESY contacts detailed probability

3.71 ILE(71)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE71 | HA | 1.00 | 0.001 | 1.00 | 0.24 |
| ILE71 | HB | 1.00 | 0.001 | 1.00 | 2.87 |
| ILE71 | HG12 | 1.00 | 0.007 | 1.00 | 0.56 |
| ILE71 | HG13 | 1.00 | 0.118 | 0.00 | 0.00 |
| ILE71 | HG21 | 1.00 | 0.042 | 0.00 | 0.00 |
| ILE71 | HD11 | 1.00 | 0.003 | 1.00 | 1.25 |
| ILE71 | H | 1.00 | 0.001 | 1.00 | -806568.00 |
| THR72 | H | 1.00 | 0.004 | 1.00 | -103999.00 |

3.71.9 Detailed Probabilities of ILE71HG12:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE71 | 1.00 | 1.00 |
| THR72 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I71HA | 1.00 |
| I71HB | 1.00 |
| I71HG13 | 1.00 |
| I71HG21 | 1.00 |
| I71HD11 | 1.00 |
| I71H | 1.00 |
| I71HG12 | 1.00 |
| T72H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE71 | HA | 1.00 | 0.017 | 1.00 | 0.29 |
| ILE71 | HB | 1.00 | 0.009 | 1.00 | 0.53 |
| ILE71 | HG12 | 1.00 | 0.012 | 1.00 | 15.92 |
| ILE71 | HG13 | 1.00 | 0.007 | 1.00 | 2.00 |
| ILE71 | HG21 | 1.00 | 0.004 | 1.00 | 0.45 |
| ILE71 | HD11 | 1.00 | 0.012 | 1.00 | 1.37 |
| ILE71 | H | 1.00 | 0.012 | 1.00 | -415117.00 |
| THR72 | H | 0.98 | 0.009 | 1.00 | -144250.00 |

3.71.10 Detailed Probabilities of ILE71HG13:

Overall probability: 0.429

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE71 | 0.43 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I71HA | 1.00 |
| I71HB | 1.00 |
| I71HG12 | 1.00 |
| I71HG21 | 1.00 |
| I71HD11 | 1.00 |
| I71H | 1.00 |
| I71HG13 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE71 | HA | 1.00 | 0.032 | 0.80 | 0.00 |
| ILE71 | HB | 1.00 | 0.037 | 0.30 | 0.00 |
| ILE71 | HG12 | 1.00 | 0.011 | 1.00 | 2.78 |
| ILE71 | HG13 | 1.00 | 0.284 | 0.00 | 0.00 |
| ILE71 | HG21 | 1.00 | 0.062 | 0.00 | 0.00 |
| ILE71 | HD11 | 1.00 | 0.037 | 0.30 | 0.00 |
| ILE71 | H | 1.00 | 0.034 | 0.60 | 0.00 |

3.71.11 Detailed Probabilities of ILE71HG21:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE71 | 0.86 | 1.00 |
| THR72 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I71HA | 1.00 |
| I71HB | 1.00 |
| I71HG12 | 1.00 |
| I71HG13 | 1.00 |
| I71HG22 | 1.00 |
| I71HD11 | 0.99 |
| I71H | 1.00 |
| T72H | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE71 | HA | 1.00 | 0.005 | 1.00 | 0.65 |
| ILE71 | HB | 1.00 | 0.000 | 1.00 | 1.21 |
| ILE71 | HG12 | 1.00 | 0.026 | 1.00 | 2.78 |
| ILE71 | HG13 | 1.00 | 0.247 | 0.00 | 0.00 |
| ILE71 | HG21 | 1.00 | 0.025 | 1.00 | 72.70 |
| ILE71 | HD11 | 0.99 | 0.000 | 1.00 | 3.08 |
| ILE71 | H | 1.00 | 0.003 | 1.00 | -575677.00 |
| THR72 | H | 0.99 | 0.002 | 1.00 | -850861.00 |
| THR72 | HA | 0.64 | 0.002 | 1.00 | 0.21 |

3.71.12 Detailed Probabilities of ILE71HD11:

Overall probability: 0.886

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE71 | 0.89 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I71HA | 0.97 |
| I71HB | 1.00 |
| I71HG12 | 1.00 |
| I71HG13 | 1.00 |
| I71HG21 | 0.99 |
| I71HD12 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE71 | HA | 0.97 | 0.008 | 1.00 | 0.34 |
| ILE71 | HB | 1.00 | 0.004 | 1.00 | 0.83 |
| ILE71 | HG12 | 1.00 | 0.031 | 0.90 | 0.00 |
| ILE71 | HG13 | 1.00 | 0.008 | 1.00 | 1.48 |
| ILE71 | HG21 | 0.99 | 0.037 | 0.30 | 0.00 |
| ILE71 | HD11 | 1.00 | 0.003 | 1.00 | 51.50 |
| ILE71 | H | 0.94 | 0.014 | 1.00 | -634581.00 |

3.71.13 Detailed Probabilities of ILE71H:

Overall probability: 0.917

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER70 | 1.00 | 0.80 |
| ILE71 | 0.86 | 1.00 |
| THR72 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| S70HA | 1.00 |
| S70HG | 0.98 |
| S70H | 1.00 |
| S70HB3 | 1.00 |
| S70HB2 | 1.00 |
| I71HA | 1.00 |
| I71HB | 1.00 |
| I71HG12 | 1.00 |
| I71HG13 | 1.00 |
| I71HG21 | 1.00 |
| I71H | 1.00 |
| T72H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER70 | HA | 1.00 | 0.008 | 1.00 | 0.90 |
| SER70 | HB2 | 1.00 | 0.007 | 1.00 | 0.45 |
| SER70 | HB3 | 1.00 | 0.008 | 1.00 | 0.34 |
| SER70 | H | 1.00 | 0.004 | 1.00 | -179463.00 |
| ILE71 | HA | 1.00 | 0.023 | 1.00 | 0.22 |
| ILE71 | HB | 1.00 | 0.007 | 1.00 | 0.38 |
| ILE71 | HG12 | 1.00 | 0.831 | 0.00 | 0.00 |
| ILE71 | HG13 | 1.00 | 0.000 | 1.00 | 0.11 |
| ILE71 | HG21 | 1.00 | 0.016 | 1.00 | 0.16 |
| ILE71 | H | 1.00 | 0.007 | 1.00 | -5820170.00 |
| ILE71 | HD11 | 0.94 | 0.010 | 1.00 | 0.26 |
| THR72 | H | 1.00 | 0.020 | 1.00 | -123043.00 |

3.72 THR(72)

Figure 62: Image from the BMRB

Residue probability: 0.906

Residue probability confidence: 0.863

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 174.404 | 174.627 | 1.788 | 0.000 | 0.000 |
| CA 3.72.1 | 62.047 | 62.330 | 4.136 | 0.900 | 0.875 |
| CB 3.72.2 | 69.485 | 69.395 | 4.500 | 0.800 | 0.833 |
| CG2 3.72.3 | 21.074 | 21.588 | 1.595 | 1.000 | 0.833 |
| N 3.72.4 | 125.574 | 115.370 | 5.913 | 1.000 | 0.909 |
| HA 3.72.5 | 5.593 | 4.461 | 0.626 | 0.750 | 0.875 |
| HB 3.72.6 | 4.281 | 4.172 | 0.855 | 1.000 | 0.833 |
| HG2 3.72.7 | 1.086 | 1.134 | 0.349 | 0.800 | 0.833 |
| H 3.72.8 | 10.252 | 8.272 | 1.597 | 1.000 | 0.909 |
| HG1 | NA | – | – | 0.000 | 0.000 |

3.72.1 Detailed Probabilities of THR72CA:

Overall probability: 0.900

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE71 | 0.50 | 1.00 |
| THR72 | 1.00 | 0.80 |
| VAL73 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I71HA | 1.00 |
| T72HB | 1.00 |
| T72HG21 | 1.00 |
| T72H | 1.00 |
| T72HG1 | 1.00 |
| T72HA | 1.00 |
| V73HA | 1.00 |
| V73H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE71 | HA | 1.00 | 0.330 | 0.00 | 0.00 |
| ILE71 | HG21 | 0.65 | 0.002 | 1.00 | 0.21 |
| THR72 | HA | 1.00 | 0.001 | 1.00 | 2.59 |
| THR72 | HB | 1.00 | 0.001 | 1.00 | 0.13 |
| THR72 | HG21 | 1.00 | 0.004 | 1.00 | 0.82 |
| THR72 | H | 1.00 | 0.001 | 1.00 | 0.15 |
| VAL73 | HA | 1.00 | 0.015 | 1.00 | 0.10 |
| VAL73 | H | 1.00 | 0.008 | 1.00 | 1.07 |
| VAL73 | HB | 0.58 | 0.006 | 1.00 | 0.09 |
| VAL73 | HG21 | 0.55 | 0.000 | 1.00 | 0.21 |

3.72.2 Detailed Probabilities of THR72CB:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR72 | 0.75 | 0.80 |
| VAL73 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T72HA | 1.00 |
| T72HG21 | 1.00 |
| T72H | 1.00 |
| T72HG1 | 1.00 |
| T72HB | 1.00 |
| V73H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR72 | HA | 1.00 | 0.003 | 1.00 | 0.14 |
| THR72 | HB | 1.00 | 0.025 | 1.00 | 19.45 |
| THR72 | HG21 | 1.00 | 0.112 | 0.00 | 0.00 |
| THR72 | H | 1.00 | 0.007 | 1.00 | 0.35 |
| VAL73 | H | 1.00 | 0.016 | 1.00 | 0.06 |

3.72.3 Detailed Probabilities of THR72CG2:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR72 | 1.00 | 0.80 |
| VAL73 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T72HA | 1.00 |
| T72HB | 1.00 |
| T72HG22 | 1.00 |
| T72H | 1.00 |
| T72HG1 | 1.00 |
| V73H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR72 | HA | 1.00 | 0.002 | 1.00 | 1.22 |
| THR72 | HB | 1.00 | 0.003 | 1.00 | 1.49 |
| THR72 | HG21 | 1.00 | 0.003 | 1.00 | 51.78 |
| THR72 | H | 1.00 | 0.009 | 1.00 | 0.19 |
| VAL73 | H | 0.97 | 0.006 | 1.00 | 0.95 |

3.72.4 Detailed Probabilities of THR72N:

Overall probability: 1.000

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE71 | 1.00 | 1.00 |
| THR72 | 1.00 | 0.80 |
| VAL73 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I71HG23 | 0.99 |
| I71H | 1.00 |
| I71HG12 | 0.98 |
| I71HA | 1.00 |
| I71HB | 1.00 |
| T72HA | 1.00 |
| T72HB | 1.00 |
| T72HG21 | 1.00 |
| T72HG1 | 1.00 |
| T72H | 1.00 |
| V73H | 1.00 |

NOESY contacts detailed probability

3.72 THR(72)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE71 | HA | 1.00 | 0.008 | 1.00 | -1572376.00 |
| ILE71 | HB | 1.00 | 0.004 | 1.00 | -103999.00 |
| ILE71 | HG12 | 0.98 | 0.009 | 1.00 | -144250.00 |
| ILE71 | HG21 | 0.99 | 0.002 | 1.00 | -850861.00 |
| ILE71 | H | 1.00 | 0.020 | 1.00 | -123043.00 |
| THR72 | HA | 1.00 | 0.004 | 1.00 | -327080.00 |
| THR72 | HB | 1.00 | 0.001 | 1.00 | -640822.00 |
| THR72 | HG21 | 1.00 | 0.007 | 1.00 | -300494.00 |
| THR72 | H | 1.00 | 0.005 | 1.00 | -4967488.00 |
| VAL73 | H | 1.00 | 0.030 | 1.00 | -123043.00 |

3.72.5 Detailed Probabilities of THR72HA:

Overall probability: 0.750

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE71 | 0.50 | 1.00 |
| THR72 | 1.00 | 0.80 |
| VAL73 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I71HA | 1.00 |
| T72HB | 1.00 |
| T72HG21 | 1.00 |
| T72H | 1.00 |
| T72HG1 | 1.00 |
| T72HA | 1.00 |
| V73HA | 1.00 |
| V73H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE71 | HA | 1.00 | 0.101 | 0.00 | 0.00 |
| ILE71 | HG21 | 0.65 | 0.002 | 1.00 | 0.08 |
| THR72 | HA | 1.00 | 0.001 | 1.00 | 2.59 |
| THR72 | HB | 1.00 | 0.003 | 1.00 | 0.14 |
| THR72 | HG21 | 1.00 | 0.002 | 1.00 | 1.22 |
| THR72 | H | 1.00 | 0.004 | 1.00 | -327080.00 |
| VAL73 | HA | 1.00 | 0.053 | 0.00 | 0.00 |
| VAL73 | H | 1.00 | 0.002 | 1.00 | -2335535.00 |

3.72.6 Detailed Probabilities of THR72HB:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR72 | 1.00 | 0.80 |
| VAL73 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T72HA | 1.00 |
| T72HG21 | 1.00 |
| T72H | 1.00 |
| T72HG1 | 1.00 |
| T72HB | 1.00 |
| V73H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR72 | HA | 1.00 | 0.001 | 1.00 | 0.13 |
| THR72 | HB | 1.00 | 0.025 | 1.00 | 19.45 |
| THR72 | HG21 | 1.00 | 0.003 | 1.00 | 1.49 |
| THR72 | H | 1.00 | 0.001 | 1.00 | -640822.00 |
| VAL73 | H | 1.00 | 0.004 | 1.00 | -131629.00 |

3.72.7 Detailed Probabilities of THR72HG21:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR72 | 0.75 | 0.80 |
| VAL73 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T72HA | 1.00 |
| T72HB | 1.00 |
| T72HG22 | 1.00 |
| T72H | 1.00 |
| T72HG1 | 1.00 |
| V73H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR72 | HA | 1.00 | 0.004 | 1.00 | 0.82 |
| THR72 | HB | 1.00 | 0.112 | 0.00 | 0.00 |
| THR72 | HG21 | 1.00 | 0.003 | 1.00 | 51.78 |
| THR72 | H | 1.00 | 0.007 | 1.00 | -300494.00 |
| VAL73 | H | 0.97 | 0.004 | 1.00 | -1366095.00 |

3.72.8 Detailed Probabilities of THR72H:

Overall probability: 1.000

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE71 | 1.00 | 1.00 |
| THR72 | 1.00 | 0.80 |
| VAL73 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I71HG23 | 0.99 |
| I71H | 1.00 |
| I71HG12 | 0.98 |
| I71HA | 1.00 |
| I71HB | 1.00 |
| T72HA | 1.00 |
| T72HB | 1.00 |
| T72HG21 | 1.00 |
| T72HG1 | 1.00 |
| T72H | 1.00 |
| V73H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE71 | HA | 1.00 | 0.008 | 1.00 | 0.77 |
| ILE71 | HB | 1.00 | 0.002 | 1.00 | 0.07 |
| ILE71 | HG12 | 0.98 | 0.000 | 1.00 | 0.06 |
| ILE71 | HG21 | 0.99 | 0.006 | 1.00 | 0.31 |
| ILE71 | H | 1.00 | 0.002 | 1.00 | -110747.00 |
| THR72 | HA | 1.00 | 0.001 | 1.00 | 0.15 |
| THR72 | HB | 1.00 | 0.007 | 1.00 | 0.35 |
| THR72 | HG21 | 1.00 | 0.009 | 1.00 | 0.19 |
| THR72 | H | 1.00 | 0.005 | 1.00 | -4967488.00 |
| VAL73 | H | 1.00 | 0.007 | 1.00 | -116050.00 |

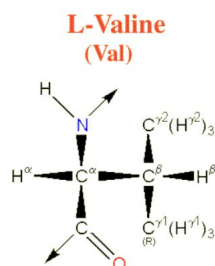
3.73 VAL(73)

Figure 63: Image from the BMRB

Residue probability: 0.665

Residue probability confidence: 0.982

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 173.754 | 175.682 | 2.367 | 0.000 | 0.000 |
| CA 3.73.1 | 61.521 | 62.613 | 4.828 | 0.667 | 1.000 |
| CB 3.73.2 | 34.387 | 32.918 | 4.591 | 0.000 | 1.000 |
| CG1 3.73.3 | 22.601 | 21.563 | 2.746 | 0.857 | 1.000 |
| CG2 3.73.4 | 22.053 | 21.368 | 2.801 | 0.800 | 1.000 |
| N 3.73.5 | 129.570 | 121.057 | 5.832 | 0.870 | 0.909 |
| HA 3.73.6 | 4.719 | 4.178 | 0.599 | 0.625 | 1.000 |
| HB 3.73.7 | 2.313 | 1.980 | 0.322 | 0.833 | 1.000 |
| HG1 3.73.8 | 1.156 | 0.816 | 0.264 | 0.500 | 1.000 |
| HG2 3.73.9 | 0.944 | 0.803 | 0.504 | 0.800 | 1.000 |
| H 3.73.10 | 9.241 | 8.311 | 0.669 | 0.700 | 0.909 |

3.73.1 Detailed Probabilities of VAL73CA:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR72 | 0.00 | 1.00 |
| VAL73 | 0.80 | 1.00 |
| THR74 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T72HA | 1.00 |
| V73HG11 | 1.00 |
| V73HG21 | 1.00 |
| V73H | 1.00 |
| V73HB | 1.00 |
| V73HA | 1.00 |
| T74H | 1.00 |
| T74HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR72 | HA | 1.00 | 0.053 | 0.00 | 0.00 |
| VAL73 | HA | 1.00 | 0.003 | 1.00 | 2.30 |
| VAL73 | HB | 1.00 | 0.021 | 1.00 | 0.23 |
| VAL73 | HG11 | 1.00 | 0.004 | 1.00 | 0.70 |
| VAL73 | HG21 | 1.00 | 0.006 | 1.00 | 0.87 |
| VAL73 | H | 1.00 | 0.116 | 0.00 | 0.00 |
| THR74 | HA | 1.00 | 0.054 | 0.00 | 0.00 |
| THR74 | H | 1.00 | 0.010 | 1.00 | 1.22 |
| THR74 | HB | 0.53 | 0.019 | 1.00 | 0.68 |

3.73.2 Detailed Probabilities of VAL73CB:

Overall probability: 0.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL73 | 0.00 | 1.00 |
| THR74 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V73HA | 1.00 |
| V73HG11 | 1.00 |
| V73HG21 | 1.00 |
| V73H | 1.00 |
| V73HB | 1.00 |
| T74H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL73 | HA | 1.00 | 3.954 | 0.00 | 0.00 |
| VAL73 | HB | 1.00 | 1.548 | 0.00 | 0.00 |
| VAL73 | HG11 | 1.00 | 0.391 | 0.00 | 0.00 |
| VAL73 | HG21 | 1.00 | 0.179 | 0.00 | 0.00 |
| VAL73 | H | 1.00 | 8.476 | 0.00 | 0.00 |
| THR74 | H | 1.00 | 8.009 | 0.00 | 0.00 |

3.73.3 Detailed Probabilities of VAL73CG1:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL73 | 0.80 | 1.00 |
| THR74 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V73HA | 1.00 |
| V73HG12 | 1.00 |
| V73HG21 | 1.00 |
| V73H | 1.00 |
| V73HB | 1.00 |
| T74H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL73 | HA | 1.00 | 0.002 | 1.00 | 0.89 |
| VAL73 | HB | 1.00 | 0.002 | 1.00 | 1.71 |
| VAL73 | HG11 | 1.00 | 0.094 | 0.00 | 0.00 |
| VAL73 | HG21 | 1.00 | 0.002 | 1.00 | 3.71 |
| VAL73 | H | 1.00 | 0.017 | 1.00 | 0.29 |
| THR74 | H | 0.97 | 0.003 | 1.00 | 1.02 |
| THR74 | HA | 0.52 | 0.005 | 1.00 | 0.11 |

3.73.4 Detailed Probabilities of VAL73CG2:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL73 | 0.80 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V73HA | 1.00 |
| V73HG11 | 1.00 |
| V73HG22 | 1.00 |
| V73H | 1.00 |
| V73HB | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL73 | HA | 1.00 | 0.178 | 0.00 | 0.00 |
| VAL73 | HB | 1.00 | 0.002 | 1.00 | 1.76 |
| VAL73 | HG11 | 1.00 | 0.003 | 1.00 | 2.97 |
| VAL73 | HG21 | 1.00 | 0.001 | 1.00 | 42.47 |
| VAL73 | H | 1.00 | 0.003 | 1.00 | 0.55 |

3.73.5 Detailed Probabilities of VAL73N:

Overall probability: 0.870

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR72 | 1.00 | 0.80 |
| VAL73 | 0.80 | 1.00 |
| THR74 | 0.70 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T72HG22 | 0.97 |
| T72HA | 1.00 |
| T72HG1 | 0.96 |
| T72HB | 1.00 |
| T72H | 1.00 |
| V73HA | 1.00 |
| V73HG11 | 1.00 |
| V73HG21 | 1.00 |
| V73HB | 1.00 |
| V73H | 1.00 |
| T74H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR72 | HA | 1.00 | 0.002 | 1.00 | -2335535.00 |
| THR72 | HB | 1.00 | 0.004 | 1.00 | -131629.00 |
| THR72 | HG21 | 0.98 | 0.004 | 1.00 | -1366095.00 |
| THR72 | H | 1.00 | 0.007 | 1.00 | -116050.00 |
| VAL73 | HA | 1.00 | 0.002 | 1.00 | -417961.00 |
| VAL73 | HB | 1.00 | 0.003 | 1.00 | -1011661.00 |
| VAL73 | HG11 | 1.00 | 0.074 | 0.00 | 0.00 |
| VAL73 | HG21 | 1.00 | 0.000 | 1.00 | -1115092.00 |
| VAL73 | H | 1.00 | 0.009 | 1.00 | -7716785.00 |
| THR74 | H | 1.00 | 0.033 | 0.70 | 0.00 |

3.73.6 Detailed Probabilities of VAL73HA:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR72 | 1.00 | 1.00 |
| VAL73 | 0.60 | 1.00 |
| THR74 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T72HA | 1.00 |
| V73HG11 | 1.00 |
| V73HG21 | 1.00 |
| V73H | 1.00 |
| V73HB | 1.00 |
| V73HA | 1.00 |
| T74H | 1.00 |
| T74HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR72 | HA | 1.00 | 0.015 | 1.00 | 0.10 |
| VAL73 | HA | 1.00 | 0.003 | 1.00 | 2.30 |
| VAL73 | HB | 1.00 | 3.954 | 0.00 | 0.00 |
| VAL73 | HG11 | 1.00 | 0.002 | 1.00 | 0.89 |
| VAL73 | HG21 | 1.00 | 0.178 | 0.00 | 0.00 |
| VAL73 | H | 1.00 | 0.002 | 1.00 | -417961.00 |
| THR74 | HA | 1.00 | 0.086 | 0.00 | 0.00 |
| THR74 | H | 1.00 | 0.005 | 1.00 | -2130336.00 |

3.73.7 Detailed Probabilities of VAL73HB:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL73 | 0.80 | 1.00 |
| THR74 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V73HA | 1.00 |
| V73HG11 | 1.00 |
| V73HG21 | 1.00 |
| V73H | 1.00 |
| V73HB | 1.00 |
| T74H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL73 | HA | 1.00 | 0.021 | 1.00 | 0.23 |
| VAL73 | HB | 1.00 | 1.548 | 0.00 | 0.00 |
| VAL73 | HG11 | 1.00 | 0.002 | 1.00 | 1.71 |
| VAL73 | HG21 | 1.00 | 0.002 | 1.00 | 1.76 |
| VAL73 | H | 1.00 | 0.003 | 1.00 | -1011661.00 |
| THR74 | H | 1.00 | 0.004 | 1.00 | -185153.00 |

3.73.8 Detailed Probabilities of VAL73HG11:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL73 | 0.40 | 1.00 |
| THR74 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V73HA | 1.00 |
| V73HG12 | 1.00 |
| V73HG21 | 1.00 |
| V73H | 1.00 |
| V73HB | 1.00 |
| T74H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL73 | HA | 1.00 | 0.004 | 1.00 | 0.70 |
| VAL73 | HB | 1.00 | 0.391 | 0.00 | 0.00 |
| VAL73 | HG11 | 1.00 | 0.094 | 0.00 | 0.00 |
| VAL73 | HG21 | 1.00 | 0.003 | 1.00 | 2.97 |
| VAL73 | H | 1.00 | 0.074 | 0.00 | 0.00 |
| THR74 | H | 0.97 | 0.004 | 1.00 | -1812448.00 |

3.73.9 Detailed Probabilities of VAL73HG21:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL73 | 0.80 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V73HA | 1.00 |
| V73HG11 | 1.00 |
| V73HG22 | 1.00 |
| V73H | 1.00 |
| V73HB | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL73 | HA | 1.00 | 0.006 | 1.00 | 0.87 |
| VAL73 | HB | 1.00 | 0.179 | 0.00 | 0.00 |
| VAL73 | HG11 | 1.00 | 0.002 | 1.00 | 3.71 |
| VAL73 | HG21 | 1.00 | 0.001 | 1.00 | 42.47 |
| VAL73 | H | 1.00 | 0.000 | 1.00 | -1115092.00 |

3.73.10 Detailed Probabilities of VAL73H:

Overall probability: 0.700

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR72 | 1.00 | 0.80 |
| VAL73 | 0.60 | 1.00 |
| THR74 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T72HG22 | 0.97 |
| T72HA | 1.00 |
| T72HG1 | 0.96 |
| T72HB | 1.00 |
| T72H | 1.00 |
| V73HA | 1.00 |
| V73HG11 | 1.00 |
| V73HG21 | 1.00 |
| V73HB | 1.00 |
| V73H | 1.00 |
| T74H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR72 | HA | 1.00 | 0.008 | 1.00 | 1.07 |
| THR72 | HB | 1.00 | 0.016 | 1.00 | 0.06 |
| THR72 | HG21 | 0.98 | 0.006 | 1.00 | 0.95 |
| THR72 | H | 1.00 | 0.030 | 1.00 | -123043.00 |
| VAL73 | HA | 1.00 | 0.116 | 0.00 | 0.00 |
| VAL73 | HB | 1.00 | 8.476 | 0.00 | 0.00 |
| VAL73 | HG11 | 1.00 | 0.017 | 1.00 | 0.29 |
| VAL73 | HG21 | 1.00 | 0.003 | 1.00 | 0.55 |
| VAL73 | H | 1.00 | 0.009 | 1.00 | -7716785.00 |
| THR74 | H | 1.00 | 0.059 | 0.00 | 0.00 |

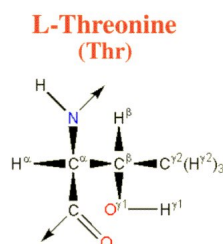
3.74 THR(74)

Figure 64: Image from the BMRB

Residue probability: 0.710

Residue probability confidence: 0.860

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 173.988 | 174.627 | 1.788 | 0.000 | 0.000 |
| CA 3.74.1 | 60.821 | 62.330 | 4.136 | 0.714 | 0.875 |
| CB 3.74.2 | 70.148 | 69.395 | 4.500 | 1.000 | 0.833 |
| CG2 3.74.3 | 20.556 | 21.588 | 1.595 | 0.210 | 0.833 |
| N 3.74.4 | 124.393 | 115.370 | 5.913 | 0.820 | 0.900 |
| HA 3.74.5 | 5.839 | 4.461 | 0.626 | 0.750 | 0.875 |
| HB 3.74.6 | 4.106 | 4.172 | 0.855 | 0.800 | 0.833 |
| HG2 3.74.7 | 1.198 | 1.134 | 0.349 | 0.640 | 0.833 |
| H 3.74.8 | 8.774 | 8.272 | 1.597 | 0.744 | 0.900 |
| HG1 | NA | – | – | 0.000 | 0.000 |

3.74.1 Detailed Probabilities of THR74CA:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL73 | 0.00 | 1.00 |
| THR74 | 1.00 | 0.80 |
| LYS75 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V73HA | 1.00 |
| T74HB | 1.00 |
| T74HG21 | 1.00 |
| T74H | 1.00 |
| T74HG1 | 1.00 |
| T74HA | 1.00 |
| K75HA | 1.00 |
| K75H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL73 | HA | 1.00 | 0.086 | 0.00 | 0.00 |
| THR74 | HA | 1.00 | 0.001 | 1.00 | 1.75 |
| THR74 | HB | 1.00 | 0.002 | 1.00 | 0.15 |
| THR74 | HG21 | 1.00 | 0.007 | 1.00 | 0.66 |
| THR74 | H | 1.00 | 0.018 | 1.00 | 0.24 |
| LYS75 | HA | 1.00 | 0.494 | 0.00 | 0.00 |
| LYS75 | H | 1.00 | 0.001 | 1.00 | 0.61 |

3.74.2 Detailed Probabilities of THR74CB:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR74 | 1.00 | 0.80 |
| LYS75 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T74HA | 1.00 |
| T74HG21 | 1.00 |
| T74H | 1.00 |
| T74HG1 | 1.00 |
| T74HB | 1.00 |
| K75H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR74 | HA | 1.00 | 0.001 | 1.00 | 0.21 |
| THR74 | HB | 1.00 | 0.001 | 1.00 | 3.20 |
| THR74 | HG21 | 1.00 | 0.005 | 1.00 | 1.29 |
| THR74 | H | 1.00 | 0.008 | 1.00 | 0.51 |
| LYS75 | H | 1.00 | 0.014 | 1.00 | 0.07 |

3.74.3 Detailed Probabilities of THR74CG2:

Overall probability: 0.210

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR74 | 0.25 | 0.80 |
| LYS75 | 0.05 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T74HA | 1.00 |
| T74HB | 1.00 |
| T74HG22 | 1.00 |
| T74H | 1.00 |
| T74HG1 | 1.00 |
| K75H | 0.96 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR74 | HA | 1.00 | 0.002 | 1.00 | 1.06 |
| THR74 | HB | 1.00 | 0.126 | 0.00 | 0.00 |
| THR74 | HG21 | 1.00 | 0.331 | 0.00 | 0.00 |
| THR74 | H | 1.00 | 0.528 | 0.00 | 0.00 |
| LYS75 | H | 0.95 | 0.117 | 0.05 | 0.00 |

3.74.4 Detailed Probabilities of THR74N:

Overall probability: 0.820

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL73 | 0.80 | 1.00 |
| THR74 | 0.80 | 0.80 |
| LYS75 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V73HA | 1.00 |
| V73H | 1.00 |
| V73HG11 | 0.97 |
| V73HB | 1.00 |
| T74HA | 1.00 |
| T74HB | 1.00 |
| T74HG21 | 1.00 |
| T74HG1 | 1.00 |
| T74H | 1.00 |
| K75H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL73 | HA | 1.00 | 0.005 | 1.00 | -2130336.00 |
| VAL73 | HB | 1.00 | 0.004 | 1.00 | -185153.00 |
| VAL73 | HG11 | 0.97 | 0.004 | 1.00 | -1812448.00 |
| VAL73 | H | 1.00 | 0.059 | 0.00 | 0.00 |
| VAL73 | HG21 | 0.94 | 0.001 | 1.00 | -588504.00 |
| THR74 | HA | 1.00 | 0.002 | 1.00 | -356788.00 |
| THR74 | HB | 1.00 | 0.001 | 1.00 | -1165926.00 |
| THR74 | HG21 | 1.00 | 0.038 | 0.20 | 0.00 |
| THR74 | H | 1.00 | 0.006 | 1.00 | -7975661.00 |
| LYS75 | H | 1.00 | 0.002 | 1.00 | -110276.00 |

3.74.5 Detailed Probabilities of THR74HA:

Overall probability: 0.750

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL73 | 0.50 | 1.00 |
| THR74 | 1.00 | 0.80 |
| LYS75 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V73HA | 1.00 |
| T74HB | 1.00 |
| T74HG21 | 1.00 |
| T74H | 1.00 |
| T74HG1 | 1.00 |
| T74HA | 1.00 |
| K75HA | 1.00 |
| K75H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL73 | HA | 1.00 | 0.054 | 0.00 | 0.00 |
| VAL73 | HG11 | 0.54 | 0.005 | 1.00 | 0.11 |
| THR74 | HA | 1.00 | 0.001 | 1.00 | 1.75 |
| THR74 | HB | 1.00 | 0.001 | 1.00 | 0.21 |
| THR74 | HG21 | 1.00 | 0.002 | 1.00 | 1.06 |
| THR74 | H | 1.00 | 0.002 | 1.00 | -356788.00 |
| LYS75 | HA | 1.00 | 0.127 | 0.00 | 0.00 |
| LYS75 | H | 1.00 | 0.001 | 1.00 | -1493524.00 |

3.74.6 Detailed Probabilities of THR74HB:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR74 | 0.75 | 0.80 |
| LYS75 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T74HA | 1.00 |
| T74HG21 | 1.00 |
| T74H | 1.00 |
| T74HG1 | 1.00 |
| T74HB | 1.00 |
| K75H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR74 | HA | 1.00 | 0.002 | 1.00 | 0.15 |
| THR74 | HB | 1.00 | 0.001 | 1.00 | 3.20 |
| THR74 | HG21 | 1.00 | 0.126 | 0.00 | 0.00 |
| THR74 | H | 1.00 | 0.001 | 1.00 | -1165926.00 |
| LYS75 | H | 1.00 | 0.005 | 1.00 | -134288.00 |

3.74.7 Detailed Probabilities of THR74HG21:

Overall probability: 0.640

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR74 | 0.55 | 0.80 |
| LYS75 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T74HA | 1.00 |
| T74HB | 1.00 |
| T74HG22 | 1.00 |
| T74H | 1.00 |
| T74HG1 | 1.00 |
| K75H | 0.96 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR74 | HA | 1.00 | 0.007 | 1.00 | 0.66 |
| THR74 | HB | 1.00 | 0.005 | 1.00 | 1.29 |
| THR74 | HG21 | 1.00 | 0.331 | 0.00 | 0.00 |
| THR74 | H | 1.00 | 0.038 | 0.20 | 0.00 |
| LYS75 | H | 0.95 | 0.008 | 1.00 | -1142098.00 |

3.74.8 Detailed Probabilities of THR74H:

Overall probability: 0.744

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL73 | 0.68 | 1.00 |
| THR74 | 0.75 | 0.80 |
| LYS75 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| V73HA | 1.00 |
| V73H | 1.00 |
| V73HG11 | 0.97 |
| V73HB | 1.00 |
| T74HA | 1.00 |
| T74HB | 1.00 |
| T74HG21 | 1.00 |
| T74HG1 | 1.00 |
| T74H | 1.00 |
| K75H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL73 | HA | 1.00 | 0.010 | 1.00 | 1.22 |
| VAL73 | HB | 1.00 | 8.009 | 0.00 | 0.00 |
| VAL73 | HG11 | 0.97 | 0.003 | 1.00 | 1.02 |
| VAL73 | H | 1.00 | 0.033 | 0.70 | 0.00 |
| THR74 | HA | 1.00 | 0.018 | 1.00 | 0.24 |
| THR74 | HB | 1.00 | 0.008 | 1.00 | 0.51 |
| THR74 | HG21 | 1.00 | 0.528 | 0.00 | 0.00 |
| THR74 | H | 1.00 | 0.006 | 1.00 | -7975661.00 |
| LYS75 | H | 1.00 | 0.015 | 1.00 | -153442.00 |

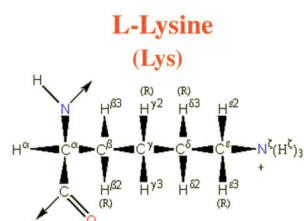


Figure 65: Image from the BMRB

Residue probability: 0.803
Residue probability confidence: 0.929

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 176.355 | 176.660 | 3.133 | 0.000 | 0.000 |
| CA 3.75.1 | 53.639 | 57.014 | 3.028 | 0.802 | 1.000 |
| CB 3.75.2 | 34.954 | 32.981 | 3.186 | 0.821 | 1.000 |
| CG 3.75.3 | 22.886 | 24.941 | 1.956 | 0.700 | 0.909 |
| CD 3.75.4 | 28.780 | 29.020 | 2.193 | 0.752 | 0.889 |
| CE 3.75.5 | 42.241 | 41.893 | 1.492 | 1.000 | 0.875 |
| N 3.75.6 | 126.207 | 120.954 | 4.210 | 1.000 | 0.909 |
| NZ | NA | - | - | 0.000 | 0.000 |
| HA 3.75.7 | 5.299 | 4.262 | 0.489 | 0.709 | 1.000 |
| HB2 3.75.8 | 1.533 | 1.774 | 0.365 | 1.000 | 1.000 |
| HB3 3.75.9 | 0.811 | 1.742 | 0.385 | 0.601 | 1.000 |
| HG 3.75.10 | 1.010 | 1.358 | 0.344 | 0.803 | 0.909 |
| HD2 3.75.11 | -0.917 | 1.614 | 0.957 | 0.891 | 0.889 |
| HD3 3.75.12 | 0.714 | 1.595 | 0.387 | 0.625 | 0.889 |
| HE2 3.75.13 | 2.350 | 2.907 | 0.230 | 0.718 | 0.875 |
| HE3 3.75.14 | 2.076 | 2.901 | 0.241 | 0.718 | 0.875 |
| H 3.75.15 | 9.472 | 8.185 | 0.605 | 0.904 | 0.909 |
| HZ | NA | - | - | 0.000 | 0.000 |

3.75.1 Detailed Probabilities of LYS75CA:

Overall probability: 0.802
Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR74 | 0.00 | 1.00 |
| LYS75 | 0.86 | 1.00 |
| GLU76 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T74HA | 1.00 |
| K75HB2 | 1.00 |
| K75HB3 | 1.00 |
| K75HG2 | 1.00 |
| K75HD2 | 0.98 |
| K75HD3 | 0.98 |
| K75H | 1.00 |
| K75HA | 1.00 |
| E76HA | 1.00 |
| E76H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR74 | HA | 1.00 | 0.127 | 0.00 | 0.00 |
| LYS75 | HA | 1.00 | 0.002 | 1.00 | 3.33 |
| LYS75 | HB2 | 1.00 | 0.001 | 1.00 | 0.52 |
| LYS75 | HB3 | 1.00 | 0.006 | 1.00 | 0.65 |
| LYS75 | HG2 | 1.00 | 0.013 | 1.00 | 0.24 |
| LYS75 | HD2 | 0.98 | 0.052 | 0.02 | 0.00 |
| LYS75 | HD3 | 0.98 | 0.002 | 1.00 | 0.08 |
| LYS75 | H | 1.00 | 0.003 | 1.00 | 0.22 |
| GLU76 | HA | 1.00 | 0.013 | 1.00 | 0.08 |
| GLU76 | H | 1.00 | 0.004 | 1.00 | 1.10 |

3.75.2 Detailed Probabilities of LYS75CB:

Overall probability: 0.821

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS75 | 0.78 | 1.00 |
| GLU76 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K75HA | 1.00 |
| K75HB3 | 1.00 |
| K75HG2 | 1.00 |
| K75HD2 | 1.00 |
| K75HD3 | 1.00 |
| K75HE2 | 0.98 |
| K75HE3 | 0.99 |
| K75H | 1.00 |
| K75HB2 | 1.00 |
| E76H | 1.00 |

NOESY contacts detailed probability

3.75 LYS(75)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS75 | HA | 1.00 | 0.003 | 1.00 | 0.41 |
| LYS75 | HB2 | 1.00 | 0.006 | 1.00 | 4.27 |
| LYS75 | HB3 | 1.00 | 0.000 | 1.00 | 0.76 |
| LYS75 | HG2 | 1.00 | 0.027 | 1.00 | 0.60 |
| LYS75 | HD2 | 1.00 | 0.001 | 1.00 | 0.16 |
| LYS75 | HD3 | 1.00 | 0.003 | 1.00 | 0.19 |
| LYS75 | HE2 | 0.98 | 0.402 | 0.02 | 0.00 |
| LYS75 | HE3 | 0.99 | 0.178 | 0.01 | 0.00 |
| LYS75 | H | 1.00 | 0.007 | 1.00 | 0.09 |
| GLU76 | H | 1.00 | 0.004 | 1.00 | 0.28 |
| GLU76 | HA | 0.65 | 0.014 | 1.00 | 0.05 |

3.75.3 Detailed Probabilities of LYS75CG:

Overall probability: 0.700

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS75 | 0.67 | 0.90 |
| GLU76 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K75HA | 1.00 |
| K75HB2 | 1.00 |
| K75HB3 | 1.00 |
| K75HG3 | 1.00 |
| K75HD2 | 1.00 |
| K75HD3 | 1.00 |
| K75HE2 | 1.00 |
| K75HE3 | 1.00 |
| K75H | 1.00 |
| K75HZ2 | 1.00 |
| E76H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS75 | HA | 1.00 | 0.004 | 1.00 | 0.13 |
| LYS75 | HB2 | 1.00 | 0.002 | 1.00 | 0.19 |
| LYS75 | HB3 | 1.00 | 0.371 | 0.00 | 0.00 |
| LYS75 | HG2 | 1.00 | 0.172 | 0.00 | 0.00 |
| LYS75 | HD2 | 1.00 | 0.007 | 1.00 | 0.18 |
| LYS75 | HD3 | 1.00 | 0.468 | 0.00 | 0.00 |
| LYS75 | HE2 | 1.00 | 0.006 | 1.00 | 0.16 |
| LYS75 | HE3 | 1.00 | 0.030 | 1.00 | 0.00 |
| LYS75 | H | 1.00 | 0.000 | 1.00 | 0.29 |
| GLU76 | H | 0.97 | 0.008 | 1.00 | 0.07 |

3.75.4 Detailed Probabilities of LYS75CD:

Overall probability: 0.752

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS75 | 0.75 | 0.89 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K75HA | 0.98 |
| K75HB2 | 1.00 |
| K75HB3 | 1.00 |
| K75HG2 | 1.00 |
| K75HD3 | 1.00 |
| K75HE2 | 1.00 |
| K75HE3 | 1.00 |
| K75HZ2 | 1.00 |
| K75HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS75 | HA | 0.98 | 2.955 | 0.02 | 0.00 |
| LYS75 | HB2 | 1.00 | 0.004 | 1.00 | 0.18 |
| LYS75 | HB3 | 1.00 | 0.090 | 0.00 | 0.00 |
| LYS75 | HG2 | 1.00 | 0.009 | 1.00 | 0.31 |
| LYS75 | HD2 | 1.00 | 0.003 | 1.00 | 0.64 |
| LYS75 | HD3 | 1.00 | 0.007 | 1.00 | 0.63 |
| LYS75 | HE2 | 1.00 | 0.006 | 1.00 | 0.15 |
| LYS75 | HE3 | 1.00 | 0.003 | 1.00 | 0.24 |

3.75.5 Detailed Probabilities of LYS75CE:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS75 | 1.00 | 0.88 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K75HB2 | 0.98 |
| K75HB3 | 0.99 |
| K75HG2 | 1.00 |
| K75HD2 | 1.00 |
| K75HD3 | 1.00 |
| K75HE3 | 1.00 |
| K75HZ2 | 1.00 |
| K75HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS75 | HB2 | 0.98 | 0.010 | 1.00 | 0.08 |
| LYS75 | HB3 | 0.99 | 0.006 | 1.00 | 0.09 |
| LYS75 | HG2 | 1.00 | 0.008 | 1.00 | 0.34 |
| LYS75 | HD2 | 1.00 | 0.002 | 1.00 | 0.32 |
| LYS75 | HD3 | 1.00 | 0.005 | 1.00 | 0.27 |
| LYS75 | HE2 | 1.00 | 0.001 | 1.00 | 1.79 |
| LYS75 | HE3 | 1.00 | 0.003 | 1.00 | 1.56 |

3.75.6 Detailed Probabilities of LYS75N:

Overall probability: 1.000

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR74 | 1.00 | 0.80 |
| LYS75 | 1.00 | 1.00 |
| GLU76 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T74H | 1.00 |
| T74HG22 | 0.95 |
| T74HG1 | 0.97 |
| T74HB | 1.00 |
| T74HA | 1.00 |
| K75HA | 1.00 |
| K75HB2 | 1.00 |
| K75HB3 | 1.00 |
| K75HG2 | 1.00 |
| K75H | 1.00 |
| E76H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR74 | HA | 1.00 | 0.001 | 1.00 | -1493524.00 |
| THR74 | HB | 1.00 | 0.005 | 1.00 | -134288.00 |
| THR74 | HG21 | 0.96 | 0.008 | 1.00 | -1142098.00 |
| THR74 | H | 1.00 | 0.015 | 1.00 | -153442.00 |
| LYS75 | HA | 1.00 | 0.005 | 1.00 | -376386.00 |
| LYS75 | HB2 | 1.00 | 0.001 | 1.00 | -271516.00 |
| LYS75 | HB3 | 1.00 | 0.003 | 1.00 | -410651.00 |
| LYS75 | HG2 | 1.00 | 0.008 | 1.00 | -1163921.00 |
| LYS75 | H | 1.00 | 0.000 | 1.00 | -3973519.00 |
| LYS75 | HD2 | 0.88 | 0.002 | 1.00 | -164169.00 |
| GLU76 | H | 1.00 | 0.000 | 1.00 | -146731.00 |

3.75.7 Detailed Probabilities of LYS75HA:

Overall probability: 0.709

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR74 | 0.00 | 1.00 |
| LYS75 | 0.73 | 1.00 |
| GLU76 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| T74HA | 1.00 |
| K75HB2 | 1.00 |
| K75HB3 | 1.00 |
| K75HG2 | 1.00 |
| K75HD2 | 0.98 |
| K75HD3 | 0.98 |
| K75H | 1.00 |
| K75HA | 1.00 |
| E76HA | 1.00 |
| E76H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR74 | HA | 1.00 | 0.494 | 0.00 | 0.00 |
| LYS75 | HA | 1.00 | 0.002 | 1.00 | 3.33 |
| LYS75 | HB2 | 1.00 | 0.003 | 1.00 | 0.41 |
| LYS75 | HB3 | 1.00 | 0.002 | 1.00 | 0.35 |
| LYS75 | HG2 | 1.00 | 0.004 | 1.00 | 0.13 |
| LYS75 | HD2 | 0.98 | 2.955 | 0.02 | 0.00 |
| LYS75 | HD3 | 0.98 | 0.515 | 0.02 | 0.00 |
| LYS75 | H | 1.00 | 0.005 | 1.00 | -376386.00 |
| LYS75 | HE2 | 0.77 | 0.033 | 0.77 | 0.00 |
| GLU76 | HA | 1.00 | 0.011 | 1.00 | 0.18 |
| GLU76 | H | 1.00 | 0.003 | 1.00 | -2829488.00 |

3.75.8 Detailed Probabilities of LYS75HB2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS75 | 1.00 | 1.00 |
| GLU76 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K75HA | 1.00 |
| K75HB3 | 1.00 |
| K75HG2 | 1.00 |
| K75HD2 | 1.00 |
| K75HD3 | 1.00 |
| K75HE2 | 0.98 |
| K75HE3 | 0.99 |
| K75H | 1.00 |
| K75HB2 | 1.00 |
| E76H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS75 | HA | 1.00 | 0.001 | 1.00 | 0.52 |
| LYS75 | HB2 | 1.00 | 0.006 | 1.00 | 4.27 |
| LYS75 | HB3 | 1.00 | 0.001 | 1.00 | 0.57 |
| LYS75 | HG2 | 1.00 | 0.002 | 1.00 | 0.19 |
| LYS75 | HD2 | 1.00 | 0.004 | 1.00 | 0.18 |
| LYS75 | HD3 | 1.00 | 0.021 | 1.00 | 0.41 |
| LYS75 | HE2 | 0.98 | 0.010 | 1.00 | 0.08 |
| LYS75 | HE3 | 0.99 | 0.003 | 1.00 | 0.08 |
| LYS75 | H | 1.00 | 0.001 | 1.00 | -271516.00 |
| GLU76 | H | 1.00 | 0.003 | 1.00 | -1255238.00 |

3.75.9 Detailed Probabilities of LYS75HB3:

Overall probability: 0.601

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS75 | 0.56 | 1.00 |
| GLU76 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K75HA | 1.00 |
| K75HB2 | 1.00 |
| K75HG2 | 1.00 |
| K75HD2 | 1.00 |
| K75HD3 | 1.00 |
| K75HE2 | 0.99 |
| K75HE3 | 0.99 |
| K75H | 1.00 |
| K75HB3 | 1.00 |
| E76H | 1.00 |

NOESY contacts detailed probability

3.75 LYS(75)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS75 | HA | 1.00 | 0.006 | 1.00 | 0.65 |
| LYS75 | HB2 | 1.00 | 0.000 | 1.00 | 0.76 |
| LYS75 | HB3 | 1.00 | 0.003 | 1.00 | 0.70 |
| LYS75 | HG2 | 1.00 | 0.371 | 0.00 | 0.00 |
| LYS75 | HD2 | 1.00 | 0.090 | 0.00 | 0.00 |
| LYS75 | HD3 | 1.00 | 0.183 | 0.00 | 0.00 |
| LYS75 | HE2 | 0.99 | 0.006 | 1.00 | 0.09 |
| LYS75 | HE3 | 0.99 | 0.088 | 0.01 | 0.00 |
| LYS75 | H | 1.00 | 0.003 | 1.00 | -410651.00 |
| GLU76 | H | 1.00 | 0.004 | 1.00 | -850114.00 |

3.75.10 Detailed Probabilities of LYS75HG2:

Overall probability: 0.803

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS75 | 0.89 | 0.90 |
| GLU76 | 0.03 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K75HA | 1.00 |
| K75HB2 | 1.00 |
| K75HB3 | 1.00 |
| K75HG3 | 1.00 |
| K75HD2 | 1.00 |
| K75HD3 | 1.00 |
| K75HE2 | 1.00 |
| K75HE3 | 1.00 |
| K75H | 1.00 |
| K75HZ2 | 1.00 |
| E76H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS75 | HA | 1.00 | 0.013 | 1.00 | 0.24 |
| LYS75 | HB2 | 1.00 | 0.027 | 1.00 | 0.60 |
| LYS75 | HB3 | 1.00 | 0.009 | 1.00 | 0.32 |
| LYS75 | HG2 | 1.00 | 0.172 | 0.00 | 0.00 |
| LYS75 | HD2 | 1.00 | 0.009 | 1.00 | 0.31 |
| LYS75 | HD3 | 1.00 | 0.016 | 1.00 | 0.28 |
| LYS75 | HE2 | 1.00 | 0.008 | 1.00 | 0.34 |
| LYS75 | HE3 | 1.00 | 0.012 | 1.00 | 0.26 |
| LYS75 | H | 1.00 | 0.008 | 1.00 | -1163921.00 |
| GLU76 | H | 0.97 | 0.048 | 0.03 | 0.00 |

3.75.11 Detailed Probabilities of LYS75HD2:

Overall probability: 0.891

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS75 | 0.89 | 0.89 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K75HA | 0.98 |
| K75HB2 | 1.00 |
| K75HB3 | 1.00 |
| K75HG2 | 1.00 |
| K75HD3 | 1.00 |
| K75HE2 | 1.00 |
| K75HE3 | 1.00 |
| K75HZ2 | 1.00 |
| K75HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS75 | HA | 0.98 | 0.052 | 0.02 | 0.00 |
| LYS75 | HB2 | 1.00 | 0.001 | 1.00 | 0.16 |
| LYS75 | HB3 | 1.00 | 0.003 | 1.00 | 0.17 |
| LYS75 | HG2 | 1.00 | 0.007 | 1.00 | 0.18 |
| LYS75 | HD2 | 1.00 | 0.003 | 1.00 | 0.64 |
| LYS75 | HD3 | 1.00 | 0.004 | 1.00 | 0.58 |
| LYS75 | HE2 | 1.00 | 0.002 | 1.00 | 0.32 |
| LYS75 | HE3 | 1.00 | 0.002 | 1.00 | 0.47 |
| LYS75 | H | 0.88 | 0.002 | 1.00 | -164169.00 |

3.75.12 Detailed Probabilities of LYS75HD3:

Overall probability: 0.625

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS75 | 0.63 | 0.89 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K75HA | 0.98 |
| K75HB2 | 1.00 |
| K75HB3 | 1.00 |
| K75HG2 | 1.00 |
| K75HD2 | 1.00 |
| K75HE2 | 1.00 |
| K75HE3 | 1.00 |
| K75HZ2 | 1.00 |
| K75HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS75 | HA | 0.98 | 0.002 | 1.00 | 0.08 |
| LYS75 | HB2 | 1.00 | 0.003 | 1.00 | 0.19 |
| LYS75 | HB3 | 1.00 | 0.094 | 0.00 | 0.00 |
| LYS75 | HG2 | 1.00 | 0.468 | 0.00 | 0.00 |
| LYS75 | HD2 | 1.00 | 0.007 | 1.00 | 0.63 |
| LYS75 | HD3 | 1.00 | 0.280 | 0.00 | 0.00 |
| LYS75 | HE2 | 1.00 | 0.005 | 1.00 | 0.27 |
| LYS75 | HE3 | 1.00 | 0.009 | 1.00 | 0.38 |

3.75.13 Detailed Probabilities of LYS75HE2:

Overall probability: 0.718

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS75 | 0.72 | 0.88 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K75HB2 | 0.98 |
| K75HB3 | 0.99 |
| K75HG2 | 1.00 |
| K75HD2 | 1.00 |
| K75HD3 | 1.00 |
| K75HE3 | 1.00 |
| K75HZ2 | 1.00 |
| K75HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS75 | HB2 | 0.98 | 0.402 | 0.02 | 0.00 |
| LYS75 | HB3 | 0.99 | 0.816 | 0.01 | 0.00 |
| LYS75 | HG2 | 1.00 | 0.006 | 1.00 | 0.16 |
| LYS75 | HD2 | 1.00 | 0.006 | 1.00 | 0.15 |
| LYS75 | HD3 | 1.00 | 0.005 | 1.00 | 0.15 |
| LYS75 | HE2 | 1.00 | 0.001 | 1.00 | 1.79 |
| LYS75 | HE3 | 1.00 | 0.000 | 1.00 | 1.59 |

3.75.14 Detailed Probabilities of LYS75HE3:

Overall probability: 0.718

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS75 | 0.72 | 0.88 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K75HB2 | 0.99 |
| K75HB3 | 0.99 |
| K75HG2 | 1.00 |
| K75HD2 | 1.00 |
| K75HD3 | 1.00 |
| K75HE2 | 1.00 |
| K75HZ2 | 1.00 |
| K75HE3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS75 | HB2 | 0.99 | 0.178 | 0.01 | 0.00 |
| LYS75 | HB3 | 0.99 | 0.542 | 0.01 | 0.00 |
| LYS75 | HG2 | 1.00 | 0.030 | 1.00 | 0.00 |
| LYS75 | HD2 | 1.00 | 0.003 | 1.00 | 0.24 |
| LYS75 | HD3 | 1.00 | 0.003 | 1.00 | 0.22 |
| LYS75 | HE2 | 1.00 | 0.003 | 1.00 | 1.56 |
| LYS75 | HE3 | 1.00 | 0.001 | 1.00 | 2.27 |

3.75.15 Detailed Probabilities of LYS75H:

Overall probability: 0.904

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR74 | 0.76 | 0.80 |
| LYS75 | 1.00 | 1.00 |
| GLU76 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T74H | 1.00 |
| T74HG22 | 0.95 |
| T74HG1 | 0.97 |
| T74HB | 1.00 |
| T74HA | 1.00 |
| K75HA | 1.00 |
| K75HB2 | 1.00 |
| K75HB3 | 1.00 |
| K75HG2 | 1.00 |
| K75H | 1.00 |
| E76H | 1.00 |

NOESY contacts detailed probability

3.75 LYS(75)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR74 | HA | 1.00 | 0.001 | 1.00 | 0.61 |
| THR74 | HB | 1.00 | 0.014 | 1.00 | 0.07 |
| THR74 | HG21 | 0.96 | 0.117 | 0.04 | 0.00 |
| THR74 | H | 1.00 | 0.002 | 1.00 | -110276.00 |
| LYS75 | HA | 1.00 | 0.003 | 1.00 | 0.22 |
| LYS75 | HB2 | 1.00 | 0.007 | 1.00 | 0.09 |
| LYS75 | HB3 | 1.00 | 0.003 | 1.00 | 0.09 |
| LYS75 | HG2 | 1.00 | 0.000 | 1.00 | 0.29 |
| LYS75 | H | 1.00 | 0.000 | 1.00 | -3973519.00 |
| GLU76 | H | 1.00 | 0.010 | 1.00 | -122692.00 |

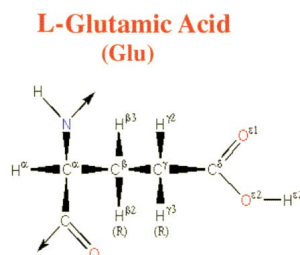
3.76 GLU(76)

Figure 66: Image from the BMRB

Residue probability: 0.915

Residue probability confidence: 0.925

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 175.080 | 176.942 | 2.547 | 0.000 | 0.000 |
| CA 3.76.1 | 59.351 | 57.442 | 3.837 | 0.889 | 1.000 |
| CB 3.76.2 | 31.094 | 30.185 | 4.018 | 0.862 | 0.875 |
| CG 3.76.3 | 35.337 | 36.085 | 1.533 | 1.000 | 0.875 |
| N 3.76.4 | 117.065 | 120.574 | 4.837 | 0.925 | 1.000 |
| HA 3.76.5 | 3.779 | 4.245 | 0.429 | 0.900 | 1.000 |
| HB2 3.76.6 | 1.897 | 2.021 | 0.233 | 1.000 | 0.875 |
| HB3 3.76.7 | 1.895 | 1.994 | 0.244 | 1.000 | 0.875 |
| HG2 3.76.8 | 2.185 | 2.258 | 0.226 | 0.786 | 0.875 |
| HG3 3.76.9 | 2.186 | 2.233 | 0.232 | 0.786 | 0.875 |
| H 3.76.10 | 8.268 | 8.332 | 0.601 | 1.000 | 1.000 |
| HE2 | NA | – | – | 0.000 | 0.000 |

3.76.1 Detailed Probabilities of GLU76CA:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS75 | 1.00 | 1.00 |
| GLU76 | 1.00 | 1.00 |
| ASN77 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K75HA | 1.00 |
| E76HB2 | 1.00 |
| E76HB3 | 1.00 |
| E76HG2 | 1.00 |
| E76HG3 | 1.00 |
| E76H | 1.00 |
| E76HA | 1.00 |
| N77HA | 1.00 |
| N77H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS75 | HA | 1.00 | 0.011 | 1.00 | 0.18 |
| GLU76 | HA | 1.00 | 0.002 | 1.00 | 10.66 |
| GLU76 | HB2 | 1.00 | 0.003 | 1.00 | 1.93 |
| GLU76 | HB3 | 1.00 | 0.005 | 1.00 | 1.93 |
| GLU76 | HG2 | 1.00 | 0.004 | 1.00 | 0.75 |
| GLU76 | HG3 | 1.00 | 0.005 | 1.00 | 0.75 |
| GLU76 | H | 1.00 | 0.002 | 1.00 | 0.83 |
| ASN77 | HA | 1.00 | 0.130 | 0.00 | 0.00 |
| ASN77 | H | 1.00 | 0.003 | 1.00 | 0.25 |

3.76.2 Detailed Probabilities of GLU76CB:

Overall probability: 0.862

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU76 | 0.82 | 0.86 |
| ASN77 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E76HA | 1.00 |
| E76HB3 | 1.00 |
| E76HG2 | 1.00 |
| E76HG3 | 1.00 |
| E76H | 1.00 |
| E76HE2 | 1.00 |
| E76HB2 | 1.00 |
| N77H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU76 | HA | 1.00 | 0.001 | 1.00 | 1.77 |
| GLU76 | HB2 | 1.00 | 0.004 | 1.00 | 92.80 |
| GLU76 | HB3 | 1.00 | 0.006 | 1.00 | 92.80 |
| GLU76 | HG2 | 1.00 | 0.035 | 0.50 | 0.00 |
| GLU76 | HG3 | 1.00 | 0.036 | 0.40 | 0.00 |
| GLU76 | H | 1.00 | 0.002 | 1.00 | 2.22 |
| ASN77 | H | 1.00 | 0.003 | 1.00 | 0.78 |
| ASN77 | HA | 0.65 | 0.010 | 1.00 | 0.09 |

3.76.3 Detailed Probabilities of GLU76CG:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU76 | 1.00 | 0.86 |
| ASN77 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E76HA | 1.00 |
| E76HB2 | 1.00 |
| E76HB3 | 1.00 |
| E76HG3 | 1.00 |
| E76H | 1.00 |
| E76HE2 | 1.00 |
| E76HG2 | 1.00 |
| N77H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU76 | HA | 1.00 | 0.005 | 1.00 | 1.18 |
| GLU76 | HB2 | 1.00 | 0.005 | 1.00 | 4.58 |
| GLU76 | HB3 | 1.00 | 0.007 | 1.00 | 4.58 |
| GLU76 | HG2 | 1.00 | 0.002 | 1.00 | 105.45 |
| GLU76 | HG3 | 1.00 | 0.003 | 1.00 | 105.45 |
| GLU76 | H | 1.00 | 0.003 | 1.00 | 1.16 |
| ASN77 | H | 0.97 | 0.004 | 1.00 | 0.38 |

3.76.4 Detailed Probabilities of GLU76N:

Overall probability: 0.925

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS75 | 0.84 | 1.00 |
| GLU76 | 1.00 | 1.00 |
| ASN77 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K75HG3 | 0.97 |
| K75HB2 | 1.00 |
| K75HA | 1.00 |
| K75H | 1.00 |
| K75HB3 | 1.00 |
| E76HA | 1.00 |
| E76HB2 | 1.00 |
| E76HB3 | 1.00 |
| E76HG2 | 1.00 |
| E76HG3 | 1.00 |
| E76H | 1.00 |
| N77H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS75 | HA | 1.00 | 0.003 | 1.00 | -2829488.00 |
| LYS75 | HB2 | 1.00 | 0.003 | 1.00 | -1255238.00 |
| LYS75 | HB3 | 1.00 | 0.004 | 1.00 | -850114.00 |
| LYS75 | HG2 | 0.98 | 0.048 | 0.02 | 0.00 |
| LYS75 | H | 1.00 | 0.010 | 1.00 | -122692.00 |
| LYS75 | HD2 | 0.59 | 0.013 | 1.00 | -83707.00 |
| GLU76 | HA | 1.00 | 0.000 | 1.00 | -1466059.00 |
| GLU76 | HB2 | 1.00 | 0.001 | 1.00 | -4261351.00 |
| GLU76 | HB3 | 1.00 | 0.003 | 1.00 | -4261351.00 |
| GLU76 | HG2 | 1.00 | 0.006 | 1.00 | -1311700.00 |
| GLU76 | HG3 | 1.00 | 0.007 | 1.00 | -1311700.00 |
| GLU76 | H | 1.00 | 0.002 | 1.00 | -13068305.00 |
| ASN77 | H | 1.00 | 0.003 | 1.00 | -793418.00 |

3.76.5 Detailed Probabilities of GLU76HA:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS75 | 1.00 | 1.00 |
| GLU76 | 1.00 | 1.00 |
| ASN77 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K75HA | 1.00 |
| E76HB2 | 1.00 |
| E76HB3 | 1.00 |
| E76HG2 | 1.00 |
| E76HG3 | 1.00 |
| E76H | 1.00 |
| E76HA | 1.00 |
| N77HA | 1.00 |
| N77H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS75 | HA | 1.00 | 0.013 | 1.00 | 0.08 |
| LYS75 | HB2 | 0.65 | 0.014 | 1.00 | 0.05 |
| GLU76 | HA | 1.00 | 0.002 | 1.00 | 10.66 |
| GLU76 | HB2 | 1.00 | 0.001 | 1.00 | 1.77 |
| GLU76 | HB3 | 1.00 | 0.001 | 1.00 | 1.77 |
| GLU76 | HG2 | 1.00 | 0.005 | 1.00 | 1.18 |
| GLU76 | HG3 | 1.00 | 0.005 | 1.00 | 1.18 |
| GLU76 | H | 1.00 | 0.000 | 1.00 | -1466059.00 |
| ASN77 | HA | 1.00 | 0.195 | 0.00 | 0.00 |
| ASN77 | H | 1.00 | 0.001 | 1.00 | -498283.00 |

3.76.6 Detailed Probabilities of GLU76HB2:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU76 | 1.00 | 0.86 |
| ASN77 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E76HA | 1.00 |
| E76HB3 | 1.00 |
| E76HG2 | 1.00 |
| E76HG3 | 1.00 |
| E76H | 1.00 |
| E76HE2 | 1.00 |
| E76HB2 | 1.00 |
| N77H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU76 | HA | 1.00 | 0.003 | 1.00 | 1.93 |
| GLU76 | HB2 | 1.00 | 0.004 | 1.00 | 92.80 |
| GLU76 | HB3 | 1.00 | 0.004 | 1.00 | 92.80 |
| GLU76 | HG2 | 1.00 | 0.005 | 1.00 | 4.58 |
| GLU76 | HG3 | 1.00 | 0.005 | 1.00 | 4.58 |
| GLU76 | H | 1.00 | 0.001 | 1.00 | -4261351.00 |
| ASN77 | H | 1.00 | 0.001 | 1.00 | -1565706.00 |

3.76.7 Detailed Probabilities of GLU76HB3:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU76 | 1.00 | 0.86 |
| ASN77 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E76HA | 1.00 |
| E76HB2 | 1.00 |
| E76HG2 | 1.00 |
| E76HG3 | 1.00 |
| E76H | 1.00 |
| E76HE2 | 1.00 |
| E76HB3 | 1.00 |
| N77H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU76 | HA | 1.00 | 0.005 | 1.00 | 1.93 |
| GLU76 | HB2 | 1.00 | 0.006 | 1.00 | 92.80 |
| GLU76 | HB3 | 1.00 | 0.006 | 1.00 | 92.80 |
| GLU76 | HG2 | 1.00 | 0.007 | 1.00 | 4.58 |
| GLU76 | HG3 | 1.00 | 0.007 | 1.00 | 4.58 |
| GLU76 | H | 1.00 | 0.003 | 1.00 | -4261351.00 |
| ASN77 | H | 1.00 | 0.001 | 1.00 | -1565706.00 |
| ASN77 | HB2 | 0.50 | 0.005 | 1.00 | 0.08 |

3.76.8 Detailed Probabilities of GLU76HG2:

Overall probability: 0.786

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU76 | 0.75 | 0.86 |
| ASN77 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E76HA | 1.00 |
| E76HB2 | 1.00 |
| E76HB3 | 1.00 |
| E76HG3 | 1.00 |
| E76H | 1.00 |
| E76HE2 | 1.00 |
| E76HG2 | 1.00 |
| N77H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU76 | HA | 1.00 | 0.005 | 1.00 | 0.75 |
| GLU76 | HB2 | 1.00 | 0.035 | 0.50 | 0.00 |
| GLU76 | HB3 | 1.00 | 0.122 | 0.00 | 0.00 |
| GLU76 | HG2 | 1.00 | 0.003 | 1.00 | 105.45 |
| GLU76 | HG3 | 1.00 | 0.003 | 1.00 | 105.45 |
| GLU76 | H | 1.00 | 0.007 | 1.00 | -1311700.00 |
| ASN77 | H | 0.97 | 0.005 | 1.00 | -459860.00 |

3.76.9 Detailed Probabilities of GLU76HG3:

Overall probability: 0.786

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU76 | 0.75 | 0.86 |
| ASN77 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E76HA | 1.00 |
| E76HB2 | 1.00 |
| E76HB3 | 1.00 |
| E76HG2 | 1.00 |
| E76H | 1.00 |
| E76HE2 | 1.00 |
| E76HG3 | 1.00 |
| N77H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU76 | HA | 1.00 | 0.005 | 1.00 | 0.75 |
| GLU76 | HB2 | 1.00 | 0.035 | 0.50 | 0.00 |
| GLU76 | HB3 | 1.00 | 0.122 | 0.00 | 0.00 |
| GLU76 | HG2 | 1.00 | 0.003 | 1.00 | 105.45 |
| GLU76 | HG3 | 1.00 | 0.003 | 1.00 | 105.45 |
| GLU76 | H | 1.00 | 0.007 | 1.00 | -1311700.00 |
| ASN77 | H | 0.97 | 0.005 | 1.00 | -459860.00 |

3.76.10 Detailed Probabilities of GLU76H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS75 | 1.00 | 1.00 |
| GLU76 | 1.00 | 1.00 |
| ASN77 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K75HG3 | 0.97 |
| K75HB2 | 1.00 |
| K75HA | 1.00 |
| K75H | 1.00 |
| K75HB3 | 1.00 |
| E76HA | 1.00 |
| E76HB2 | 1.00 |
| E76HB3 | 1.00 |
| E76HG2 | 1.00 |
| E76HG3 | 1.00 |
| E76H | 1.00 |
| N77H | 1.00 |

NOESY contacts detailed probability

3.76 GLU(76)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS75 | HA | 1.00 | 0.004 | 1.00 | 1.10 |
| LYS75 | HB2 | 1.00 | 0.004 | 1.00 | 0.28 |
| LYS75 | HB3 | 1.00 | 0.004 | 1.00 | 0.21 |
| LYS75 | HG2 | 0.98 | 0.008 | 1.00 | 0.07 |
| LYS75 | H | 1.00 | 0.000 | 1.00 | -146731.00 |
| GLU76 | HA | 1.00 | 0.002 | 1.00 | 0.83 |
| GLU76 | HB2 | 1.00 | 0.002 | 1.00 | 2.22 |
| GLU76 | HB3 | 1.00 | 0.002 | 1.00 | 2.22 |
| GLU76 | HG2 | 1.00 | 0.003 | 1.00 | 1.16 |
| GLU76 | HG3 | 1.00 | 0.003 | 1.00 | 1.16 |
| GLU76 | H | 1.00 | 0.002 | 1.00 | -13068305.00 |
| ASN77 | H | 1.00 | 0.001 | 1.00 | -878518.00 |
| ASN77 | HA | 0.83 | 0.001 | 1.00 | 1.00 |

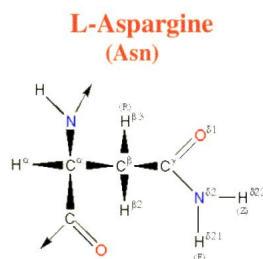
3.77 ASN(77)

Figure 67: Image from the BMRB

Residue probability: 0.951

Residue probability confidence: 0.918

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|--------------|-------------|---------|--------|---------------------|--------------------|
| C | NA | – | – | 0.000 | 0.000 |
| CA 3.77.1 | 52.289 | 53.674 | 5.429 | 0.780 | 0.889 |
| CB 3.77.2 | 39.917 | 38.785 | 5.449 | 1.000 | 0.857 |
| N 3.77.3 | 108.144 | 118.907 | 6.480 | 1.000 | 0.917 |
| ND2 3.77.4 | 113.737 | 112.932 | 14.355 | 1.000 | 1.000 |
| HA 3.77.5 | 4.682 | 4.658 | 0.371 | 0.900 | 0.889 |
| HB2 3.77.6 | 2.908 | 2.800 | 0.341 | 1.000 | 0.857 |
| HB3 3.77.7 | 3.038 | 2.739 | 0.364 | 1.000 | 0.857 |
| H 3.77.8 | 7.040 | 8.328 | 0.633 | 1.000 | 0.917 |
| HD21 3.77.9 | 7.643 | 7.343 | 1.188 | 0.833 | 1.000 |
| HD22 3.77.10 | 6.805 | 7.145 | 1.184 | 1.000 | 1.000 |

3.77.1 Detailed Probabilities of ASN77CA:

Overall probability: 0.780

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU76 | 0.65 | 1.00 |
| ASN77 | 0.83 | 1.00 |
| GLU78 | 1.00 | 0.50 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E76HA | 1.00 |
| N77HB2 | 1.00 |
| N77HB3 | 1.00 |
| N77H | 1.00 |
| N77HD21 | 1.00 |
| N77HD22 | 1.00 |
| N77HA | 1.00 |
| E78H | 1.00 |
| E78HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU76 | HA | 1.00 | 0.195 | 0.00 | 0.00 |
| GLU76 | HB2 | 0.65 | 0.032 | 0.80 | 0.00 |
| GLU76 | HB3 | 0.78 | 0.034 | 0.78 | 0.00 |
| GLU76 | H | 0.83 | 0.001 | 1.00 | 1.00 |
| ASN77 | HA | 1.00 | 0.002 | 1.00 | 9.08 |
| ASN77 | HB2 | 1.00 | 0.006 | 1.00 | 1.27 |
| ASN77 | HB3 | 1.00 | 0.004 | 1.00 | 1.05 |
| ASN77 | H | 1.00 | 0.001 | 1.00 | 0.82 |
| ASN77 | HD21 | 1.00 | 0.215 | 0.00 | 0.00 |
| ASN77 | HD22 | 1.00 | 0.023 | 1.00 | 0.28 |
| GLU78 | HA | 1.00 | 0.018 | 1.00 | 0.19 |

3.77.2 Detailed Probabilities of ASN77CB:

Overall probability: 1.000

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN77 | 1.00 | 1.00 |
| GLU78 | 0.00 | 0.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N77HA | 1.00 |
| N77HB3 | 1.00 |
| N77H | 1.00 |
| N77HD21 | 1.00 |
| N77HD22 | 1.00 |
| N77HB2 | 1.00 |
| E78H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN77 | HA | 1.00 | 0.002 | 1.00 | 0.65 |
| ASN77 | HB2 | 1.00 | 0.002 | 1.00 | 6.04 |
| ASN77 | HB3 | 1.00 | 0.003 | 1.00 | 3.43 |
| ASN77 | H | 1.00 | 0.002 | 1.00 | 0.23 |
| ASN77 | HD21 | 1.00 | 0.004 | 1.00 | 0.38 |
| ASN77 | HD22 | 1.00 | 0.006 | 1.00 | 0.15 |

3.77.3 Detailed Probabilities of ASN77N:

Overall probability: 1.000

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU76 | 1.00 | 1.00 |
| ASN77 | 1.00 | 1.00 |
| GLU78 | NaN | 0.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E76HG2 | 0.98 |
| E76HB3 | 1.00 |
| E76HG3 | 0.97 |
| E76HB2 | 1.00 |
| E76HA | 1.00 |
| E76H | 1.00 |
| N77HA | 1.00 |
| N77HB2 | 1.00 |
| N77HB3 | 1.00 |
| N77HD21 | 0.98 |
| N77H | 1.00 |
| E78H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU76 | HA | 1.00 | 0.001 | 1.00 | -498283.00 |
| GLU76 | HB2 | 1.00 | 0.001 | 1.00 | -1565706.00 |
| GLU76 | HB3 | 1.00 | 0.001 | 1.00 | -1565706.00 |
| GLU76 | HG2 | 0.98 | 0.004 | 1.00 | -459860.00 |
| GLU76 | HG3 | 0.97 | 0.005 | 1.00 | -459860.00 |
| GLU76 | H | 1.00 | 0.001 | 1.00 | -878518.00 |
| ASN77 | HA | 1.00 | 0.001 | 1.00 | -785471.00 |
| ASN77 | HB2 | 1.00 | 0.002 | 1.00 | -360820.00 |
| ASN77 | HB3 | 1.00 | 0.003 | 1.00 | -385405.00 |
| ASN77 | H | 1.00 | 0.002 | 1.00 | -13856290.00 |
| ASN77 | HD21 | 0.98 | 0.001 | 1.00 | -106673.00 |
| ASN77 | HD22 | 0.63 | 0.001 | 1.00 | -128406.00 |

3.77.4 Detailed Probabilities of ASN77ND2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN77 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N77HA | 1.00 |
| N77HB2 | 1.00 |
| N77HB3 | 1.00 |
| N77H | 0.98 |
| N77HD22 | 1.00 |
| N77HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN77 | HA | 1.00 | 0.006 | 1.00 | -265530.00 |
| ASN77 | HB2 | 1.00 | 0.001 | 1.00 | -639218.00 |
| ASN77 | HB3 | 1.00 | 0.002 | 1.00 | -1011561.00 |
| ASN77 | H | 0.98 | 0.010 | 1.00 | -184757.00 |
| ASN77 | HD21 | 1.00 | 0.002 | 1.00 | -12536101.00 |
| ASN77 | HD22 | 1.00 | 0.001 | 1.00 | -9958766.00 |

3.77.5 Detailed Probabilities of ASN77HA:

Overall probability: 0.900

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU76 | 0.67 | 1.00 |
| ASN77 | 1.00 | 1.00 |
| GLU78 | 1.00 | 0.50 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E76HA | 1.00 |
| N77HB2 | 1.00 |
| N77HB3 | 1.00 |
| N77H | 1.00 |
| N77HD21 | 1.00 |
| N77HD22 | 1.00 |
| N77HA | 1.00 |
| E78H | 1.00 |
| E78HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU76 | HA | 1.00 | 0.130 | 0.00 | 0.00 |
| GLU76 | HB2 | 0.65 | 0.010 | 1.00 | 0.09 |
| GLU76 | HB3 | 0.78 | 0.010 | 1.00 | 0.09 |
| ASN77 | HA | 1.00 | 0.002 | 1.00 | 9.08 |
| ASN77 | HB2 | 1.00 | 0.002 | 1.00 | 0.65 |
| ASN77 | HB3 | 1.00 | 0.009 | 1.00 | 0.76 |
| ASN77 | H | 1.00 | 0.001 | 1.00 | -785471.00 |
| ASN77 | HD21 | 1.00 | 0.006 | 1.00 | -265530.00 |
| ASN77 | HD22 | 1.00 | 0.000 | 1.00 | -149332.00 |
| GLU78 | HA | 1.00 | 0.003 | 1.00 | 0.09 |

3.77.6 Detailed Probabilities of ASN77HB2:

Overall probability: 1.000

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN77 | 1.00 | 1.00 |
| GLU78 | 0.00 | 0.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N77HA | 1.00 |
| N77HB3 | 1.00 |
| N77H | 1.00 |
| N77HD21 | 1.00 |
| N77HD22 | 1.00 |
| N77HB2 | 1.00 |
| E78H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN77 | HA | 1.00 | 0.006 | 1.00 | 1.27 |
| ASN77 | HB2 | 1.00 | 0.002 | 1.00 | 6.04 |
| ASN77 | HB3 | 1.00 | 0.008 | 1.00 | 3.64 |
| ASN77 | H | 1.00 | 0.002 | 1.00 | -360820.00 |
| ASN77 | HD21 | 1.00 | 0.001 | 1.00 | -639218.00 |
| ASN77 | HD22 | 1.00 | 0.004 | 1.00 | -405460.00 |

3.77.7 Detailed Probabilities of ASN77HB3:

Overall probability: 1.000

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN77 | 1.00 | 1.00 |
| GLU78 | 0.00 | 0.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N77HA | 1.00 |
| N77HB2 | 1.00 |
| N77H | 1.00 |
| N77HD21 | 1.00 |
| N77HD22 | 1.00 |
| N77HB3 | 1.00 |
| E78H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN77 | HA | 1.00 | 0.004 | 1.00 | 1.05 |
| ASN77 | HB2 | 1.00 | 0.003 | 1.00 | 3.43 |
| ASN77 | HB3 | 1.00 | 0.018 | 1.00 | 6.62 |
| ASN77 | H | 1.00 | 0.003 | 1.00 | -385405.00 |
| ASN77 | HD21 | 1.00 | 0.002 | 1.00 | -1011561.00 |
| ASN77 | HD22 | 1.00 | 0.003 | 1.00 | -670967.00 |

3.77.8 Detailed Probabilities of ASN77H:

Overall probability: 1.000

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU76 | 1.00 | 1.00 |
| ASN77 | 1.00 | 1.00 |
| GLU78 | NaN | 0.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E76HG2 | 0.98 |
| E76HB3 | 1.00 |
| E76HG3 | 0.97 |
| E76HB2 | 1.00 |
| E76HA | 1.00 |
| E76H | 1.00 |
| N77HA | 1.00 |
| N77HB2 | 1.00 |
| N77HB3 | 1.00 |
| N77HD21 | 0.98 |
| N77H | 1.00 |
| E78H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU76 | HA | 1.00 | 0.003 | 1.00 | 0.25 |
| GLU76 | HB2 | 1.00 | 0.003 | 1.00 | 0.78 |
| GLU76 | HB3 | 1.00 | 0.003 | 1.00 | 0.78 |
| GLU76 | HG2 | 0.98 | 0.004 | 1.00 | 0.38 |
| GLU76 | HG3 | 0.97 | 0.004 | 1.00 | 0.38 |
| GLU76 | H | 1.00 | 0.003 | 1.00 | -793418.00 |
| ASN77 | HA | 1.00 | 0.001 | 1.00 | 0.82 |
| ASN77 | HB2 | 1.00 | 0.002 | 1.00 | 0.23 |
| ASN77 | HB3 | 1.00 | 0.006 | 1.00 | 0.24 |
| ASN77 | H | 1.00 | 0.002 | 1.00 | -13856290.00 |
| ASN77 | HD21 | 0.98 | 0.010 | 1.00 | -184757.00 |
| ASN77 | HD22 | 0.63 | 0.016 | 1.00 | -293659.00 |

3.77.9 Detailed Probabilities of ASN77HD21:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN77 | 0.83 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N77HA | 1.00 |
| N77HB2 | 1.00 |
| N77HB3 | 1.00 |
| N77H | 0.98 |
| N77HD22 | 1.00 |
| N77HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN77 | HA | 1.00 | 0.215 | 0.00 | 0.00 |
| ASN77 | HB2 | 1.00 | 0.004 | 1.00 | 0.38 |
| ASN77 | HB3 | 1.00 | 0.000 | 1.00 | 0.49 |
| ASN77 | H | 0.98 | 0.001 | 1.00 | -106673.00 |
| ASN77 | HD21 | 1.00 | 0.002 | 1.00 | -12536101.00 |
| ASN77 | HD22 | 1.00 | 0.002 | 1.00 | -11255001.00 |

3.77.10 Detailed Probabilities of ASN77HD22:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN77 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N77HA | 1.00 |
| N77HB2 | 1.00 |
| N77HB3 | 1.00 |
| N77HD21 | 1.00 |
| N77HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN77 | HA | 1.00 | 0.023 | 1.00 | 0.28 |
| ASN77 | HB2 | 1.00 | 0.006 | 1.00 | 0.15 |
| ASN77 | HB3 | 1.00 | 0.007 | 1.00 | 0.20 |
| ASN77 | HD21 | 1.00 | 0.001 | 1.00 | -9958766.00 |
| ASN77 | HD22 | 1.00 | 0.004 | 1.00 | -16362167.00 |
| ASN77 | H | 0.63 | 0.001 | 1.00 | -128406.00 |

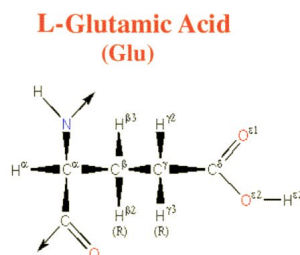
3.78 GLU(78)

Figure 68: Image from the BMRB

Residue probability: 0.719

Residue probability confidence: 0.785

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 176.407 | 176.942 | 2.547 | 0.000 | 0.000 |
| CA 3.78.1 | 58.612 | 57.442 | 3.837 | 0.625 | 0.889 |
| CB 3.78.2 | 29.862 | 30.185 | 4.018 | 1.000 | 0.750 |
| CG 3.78.3 | 36.645 | 36.085 | 1.533 | 0.500 | 0.750 |
| N | NA | – | – | 0.000 | 0.000 |
| HA 3.78.4 | 4.022 | 4.245 | 0.429 | 0.625 | 0.889 |
| HB2 3.78.5 | 2.066 | 2.021 | 0.233 | 0.833 | 0.750 |
| HB3 3.78.6 | 2.067 | 1.994 | 0.244 | 0.833 | 0.750 |
| HG2 3.78.7 | 2.331 | 2.258 | 0.226 | 0.667 | 0.750 |
| HG3 3.78.8 | 2.328 | 2.233 | 0.232 | 0.667 | 0.750 |
| H | NA | – | – | 0.000 | 0.000 |
| HE2 | NA | – | – | 0.000 | 0.000 |

3.78.1 Detailed Probabilities of GLU78CA:

Overall probability: 0.625

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN77 | 1.00 | 1.00 |
| GLU78 | 0.80 | 0.83 |
| GLU79 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| N77HA | 1.00 |
| E78HB2 | 1.00 |
| E78HB3 | 1.00 |
| E78HG2 | 1.00 |
| E78HG3 | 1.00 |
| E78H | 1.00 |
| E78HA | 1.00 |
| E79H | 1.00 |
| E79HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN77 | HA | 1.00 | 0.003 | 1.00 | 0.09 |
| GLU78 | HA | 1.00 | 0.358 | 0.00 | 0.00 |
| GLU78 | HB2 | 1.00 | 0.002 | 1.00 | 2.76 |
| GLU78 | HB3 | 1.00 | 0.003 | 1.00 | 2.76 |
| GLU78 | HG2 | 1.00 | 0.010 | 1.00 | 0.81 |
| GLU78 | HG3 | 1.00 | 0.007 | 1.00 | 0.81 |
| GLU79 | HA | 1.00 | 0.339 | 0.00 | 0.00 |
| GLU79 | H | 1.00 | 0.114 | 0.00 | 0.00 |

3.78.2 Detailed Probabilities of GLU78CB:

Overall probability: 1.000

Overall confidence: 0.750

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU78 | 1.00 | 0.71 |
| GLU79 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E78HA | 1.00 |
| E78HB3 | 1.00 |
| E78HG2 | 1.00 |
| E78HG3 | 1.00 |
| E78H | 1.00 |
| E78HE2 | 1.00 |
| E78HB2 | 1.00 |
| E79H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU78 | HA | 1.00 | 0.001 | 1.00 | 1.62 |
| GLU78 | HB2 | 1.00 | 0.005 | 1.00 | 28.37 |
| GLU78 | HB3 | 1.00 | 0.006 | 1.00 | 28.37 |
| GLU78 | HG2 | 1.00 | 0.013 | 1.00 | 2.24 |
| GLU78 | HG3 | 1.00 | 0.010 | 1.00 | 2.24 |
| GLU79 | H | 1.00 | 0.004 | 1.00 | 0.38 |
| GLU79 | HA | 0.69 | 0.020 | 1.00 | 1.62 |

3.78.3 Detailed Probabilities of GLU78CG:

Overall probability: 0.500

Overall confidence: 0.750

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU78 | 0.40 | 0.71 |
| GLU79 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E78HA | 1.00 |
| E78HB2 | 1.00 |
| E78HB3 | 1.00 |
| E78HG3 | 1.00 |
| E78H | 1.00 |
| E78HE2 | 1.00 |
| E78HG2 | 1.00 |
| E79H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU78 | HA | 1.00 | 0.145 | 0.00 | 0.00 |
| GLU78 | HB2 | 1.00 | 0.001 | 1.00 | 3.52 |
| GLU78 | HB3 | 1.00 | 0.002 | 1.00 | 3.52 |
| GLU78 | HG2 | 1.00 | 0.266 | 0.00 | 0.00 |
| GLU78 | HG3 | 1.00 | 0.263 | 0.00 | 0.00 |
| GLU79 | H | 0.98 | 0.030 | 1.00 | 0.00 |

3.78.4 Detailed Probabilities of GLU78HA:

Overall probability: 0.625

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN77 | 1.00 | 1.00 |
| GLU78 | 0.40 | 0.83 |
| GLU79 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| N77HA | 1.00 |
| E78HB2 | 1.00 |
| E78HB3 | 1.00 |
| E78HG2 | 1.00 |
| E78HG3 | 1.00 |
| E78H | 1.00 |
| E78HA | 1.00 |
| E79H | 1.00 |
| E79HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN77 | HA | 1.00 | 0.018 | 1.00 | 0.19 |
| GLU78 | HA | 1.00 | 0.358 | 0.00 | 0.00 |
| GLU78 | HB2 | 1.00 | 0.001 | 1.00 | 1.62 |
| GLU78 | HB3 | 1.00 | 0.001 | 1.00 | 1.62 |
| GLU78 | HG2 | 1.00 | 0.145 | 0.00 | 0.00 |
| GLU78 | HG3 | 1.00 | 0.145 | 0.00 | 0.00 |
| GLU79 | HA | 1.00 | 0.022 | 1.00 | 36.36 |
| GLU79 | H | 1.00 | 0.015 | 1.00 | -2159032.00 |

3.78.5 Detailed Probabilities of GLU78HB2:

Overall probability: 0.833

Overall confidence: 0.750

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU78 | 1.00 | 0.71 |
| GLU79 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E78HA | 1.00 |
| E78HB3 | 1.00 |
| E78HG2 | 1.00 |
| E78HG3 | 1.00 |
| E78H | 1.00 |
| E78HE2 | 1.00 |
| E78HB2 | 1.00 |
| E79H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU78 | HA | 1.00 | 0.002 | 1.00 | 2.76 |
| GLU78 | HB2 | 1.00 | 0.005 | 1.00 | 28.37 |
| GLU78 | HB3 | 1.00 | 0.005 | 1.00 | 28.37 |
| GLU78 | HG2 | 1.00 | 0.001 | 1.00 | 3.52 |
| GLU78 | HG3 | 1.00 | 0.001 | 1.00 | 3.52 |
| GLU79 | H | 1.00 | 0.051 | 0.00 | 0.00 |

3.78.6 Detailed Probabilities of GLU78HB3:

Overall probability: 0.833

Overall confidence: 0.750

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU78 | 1.00 | 0.71 |
| GLU79 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E78HA | 1.00 |
| E78HB2 | 1.00 |
| E78HG2 | 1.00 |
| E78HG3 | 1.00 |
| E78H | 1.00 |
| E78HE2 | 1.00 |
| E78HB3 | 1.00 |
| E79H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU78 | HA | 1.00 | 0.003 | 1.00 | 2.76 |
| GLU78 | HB2 | 1.00 | 0.006 | 1.00 | 28.37 |
| GLU78 | HB3 | 1.00 | 0.006 | 1.00 | 28.37 |
| GLU78 | HG2 | 1.00 | 0.002 | 1.00 | 3.52 |
| GLU78 | HG3 | 1.00 | 0.002 | 1.00 | 3.52 |
| GLU79 | H | 1.00 | 0.052 | 0.00 | 0.00 |

3.78.7 Detailed Probabilities of GLU78HG2:

Overall probability: 0.667

Overall confidence: 0.750

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU78 | 0.60 | 0.71 |
| GLU79 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E78HA | 1.00 |
| E78HB2 | 1.00 |
| E78HB3 | 1.00 |
| E78HG3 | 1.00 |
| E78H | 1.00 |
| E78HE2 | 1.00 |
| E78HG2 | 1.00 |
| E79H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU78 | HA | 1.00 | 0.010 | 1.00 | 0.81 |
| GLU78 | HB2 | 1.00 | 0.013 | 1.00 | 2.24 |
| GLU78 | HB3 | 1.00 | 0.013 | 1.00 | 2.24 |
| GLU78 | HG2 | 1.00 | 0.266 | 0.00 | 0.00 |
| GLU78 | HG3 | 1.00 | 0.266 | 0.00 | 0.00 |
| GLU79 | H | 0.98 | 0.002 | 1.00 | -320469.00 |

3.78.8 Detailed Probabilities of GLU78HG3:

Overall probability: 0.667

Overall confidence: 0.750

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU78 | 0.60 | 0.71 |
| GLU79 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E78HA | 1.00 |
| E78HB2 | 1.00 |
| E78HB3 | 1.00 |
| E78HG2 | 1.00 |
| E78H | 1.00 |
| E78HE2 | 1.00 |
| E78HG3 | 1.00 |
| E79H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU78 | HA | 1.00 | 0.007 | 1.00 | 0.81 |
| GLU78 | HB2 | 1.00 | 0.010 | 1.00 | 2.24 |
| GLU78 | HB3 | 1.00 | 0.010 | 1.00 | 2.24 |
| GLU78 | HG2 | 1.00 | 0.263 | 0.00 | 0.00 |
| GLU78 | HG3 | 1.00 | 0.263 | 0.00 | 0.00 |
| GLU79 | H | 0.97 | 0.005 | 1.00 | -320469.00 |

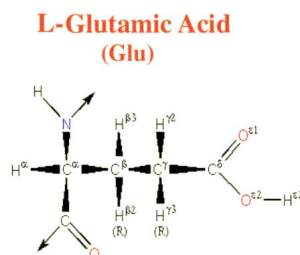
3.79 GLU(79)

Figure 69: Image from the BMRB

Residue probability: 0.811

Residue probability confidence: 0.910

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 176.849 | 176.942 | 2.547 | 0.000 | 0.000 |
| CA 3.79.1 | 57.741 | 57.442 | 3.837 | 0.889 | 1.000 |
| CB 3.79.2 | 28.980 | 30.185 | 4.018 | 0.714 | 0.875 |
| CG 3.79.3 | 36.541 | 36.085 | 1.533 | 0.857 | 0.875 |
| N 3.79.4 | 117.872 | 120.574 | 4.837 | 0.857 | 0.923 |
| HA 3.79.5 | 4.003 | 4.245 | 0.429 | 0.636 | 1.000 |
| HB2 3.79.6 | 2.010 | 2.021 | 0.233 | 0.429 | 0.875 |
| HB3 3.79.7 | 1.935 | 1.994 | 0.244 | 0.875 | 0.875 |
| HG2 3.79.8 | 2.229 | 2.258 | 0.226 | 1.000 | 0.875 |
| HG3 3.79.9 | 2.230 | 2.233 | 0.232 | 1.000 | 0.875 |
| H 3.79.10 | 8.370 | 8.332 | 0.601 | 0.857 | 0.923 |
| HE2 | NA | – | – | 0.000 | 0.000 |

3.79.1 Detailed Probabilities of GLU79CA:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU78 | 1.00 | 1.00 |
| GLU79 | 0.83 | 1.00 |
| LEU80 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E78HA | 1.00 |
| E79HB2 | 1.00 |
| E79HB3 | 1.00 |
| E79HG2 | 1.00 |
| E79HG3 | 1.00 |
| E79H | 1.00 |
| E79HA | 1.00 |
| L80H | 1.00 |
| L80HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU78 | HA | 1.00 | 0.022 | 1.00 | 36.36 |
| GLU79 | HA | 1.00 | 0.003 | 1.00 | 36.36 |
| GLU79 | HB2 | 1.00 | 0.012 | 1.00 | 2.52 |
| GLU79 | HB3 | 1.00 | 0.063 | 0.00 | 0.00 |
| GLU79 | HG2 | 1.00 | 0.001 | 1.00 | 2.15 |
| GLU79 | HG3 | 1.00 | 0.000 | 1.00 | 2.15 |
| GLU79 | H | 1.00 | 0.003 | 1.00 | 1.47 |
| LEU80 | HA | 1.00 | 0.004 | 1.00 | 0.23 |
| LEU80 | H | 1.00 | 0.026 | 1.00 | 0.64 |

3.79.2 Detailed Probabilities of GLU79CB:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU79 | 0.67 | 0.86 |
| LEU80 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E79HA | 1.00 |
| E79HB3 | 1.00 |
| E79HG2 | 1.00 |
| E79HG3 | 1.00 |
| E79H | 1.00 |
| E79HE2 | 1.00 |
| E79HB2 | 1.00 |
| L80H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU79 | HA | 1.00 | 0.138 | 0.00 | 0.00 |
| GLU79 | HB2 | 1.00 | 0.060 | 0.00 | 0.00 |
| GLU79 | HB3 | 1.00 | 0.015 | 1.00 | 18.54 |
| GLU79 | HG2 | 1.00 | 0.010 | 1.00 | 2.72 |
| GLU79 | HG3 | 1.00 | 0.011 | 1.00 | 2.72 |
| GLU79 | H | 1.00 | 0.008 | 1.00 | 0.73 |
| LEU80 | H | 1.00 | 0.000 | 1.00 | 0.26 |

3.79.3 Detailed Probabilities of GLU79CG:

Overall probability: 0.857

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU79 | 0.83 | 0.86 |
| LEU80 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E79HA | 1.00 |
| E79HB2 | 1.00 |
| E79HB3 | 1.00 |
| E79HG3 | 1.00 |
| E79H | 1.00 |
| E79HE2 | 1.00 |
| E79HG2 | 1.00 |
| L80H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU79 | HA | 1.00 | 0.019 | 1.00 | 1.51 |
| GLU79 | HB2 | 1.00 | 0.061 | 0.00 | 0.00 |
| GLU79 | HB3 | 1.00 | 0.012 | 1.00 | 3.05 |
| GLU79 | HG2 | 1.00 | 0.009 | 1.00 | 180.23 |
| GLU79 | HG3 | 1.00 | 0.010 | 1.00 | 180.23 |
| GLU79 | H | 1.00 | 0.008 | 1.00 | 0.77 |
| LEU80 | H | 0.97 | 0.017 | 1.00 | 0.17 |

3.79.4 Detailed Probabilities of GLU79N:

Overall probability: 0.857

Overall confidence: 0.923

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU78 | 0.60 | 0.83 |
| GLU79 | 1.00 | 1.00 |
| LEU80 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E78HG2 | 0.98 |
| E78HA | 1.00 |
| E78H | 1.00 |
| E78HB3 | 1.00 |
| E78HG3 | 0.97 |
| E78HB2 | 1.00 |
| E79HA | 1.00 |
| E79HB2 | 1.00 |
| E79HB3 | 1.00 |
| E79HG2 | 1.00 |
| E79HG3 | 1.00 |
| E79H | 1.00 |
| L80H | 1.00 |

NOESY contacts detailed probability

3.79 GLU(79)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU78 | HA | 1.00 | 0.015 | 1.00 | -2159032.00 |
| GLU78 | HB2 | 1.00 | 0.051 | 0.00 | 0.00 |
| GLU78 | HB3 | 1.00 | 0.052 | 0.00 | 0.00 |
| GLU78 | HG2 | 0.98 | 0.002 | 1.00 | -320469.00 |
| GLU78 | HG3 | 0.97 | 0.005 | 1.00 | -320469.00 |
| GLU79 | HA | 1.00 | 0.004 | 1.00 | -2159032.00 |
| GLU79 | HB2 | 1.00 | 0.005 | 1.00 | -1788928.00 |
| GLU79 | HB3 | 1.00 | 0.009 | 1.00 | -2408894.00 |
| GLU79 | HG2 | 1.00 | 0.003 | 1.00 | -1654494.00 |
| GLU79 | HG3 | 1.00 | 0.004 | 1.00 | -1654494.00 |
| GLU79 | H | 1.00 | 0.003 | 1.00 | -15771137.00 |
| LEU80 | H | 1.00 | 0.000 | 1.00 | -2754307.00 |
| LEU80 | HA | 0.93 | 0.007 | 1.00 | -180036.00 |
| LEU80 | HB2 | 0.69 | 0.002 | 1.00 | -232805.00 |

3.79.5 Detailed Probabilities of GLU79HA:

Overall probability: 0.636

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU78 | 0.67 | 1.00 |
| GLU79 | 0.67 | 1.00 |
| LEU80 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E78HA | 1.00 |
| E79HB2 | 1.00 |
| E79HB3 | 1.00 |
| E79HG2 | 1.00 |
| E79HG3 | 1.00 |
| E79H | 1.00 |
| E79HA | 1.00 |
| L80H | 1.00 |
| L80HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU78 | HA | 1.00 | 0.339 | 0.00 | 0.00 |
| GLU78 | HB2 | 0.69 | 0.020 | 1.00 | 1.62 |
| GLU78 | HB3 | 0.81 | 0.020 | 1.00 | 1.62 |
| GLU79 | HA | 1.00 | 0.003 | 1.00 | 36.36 |
| GLU79 | HB2 | 1.00 | 0.138 | 0.00 | 0.00 |
| GLU79 | HB3 | 1.00 | 1.781 | 0.00 | 0.00 |
| GLU79 | HG2 | 1.00 | 0.019 | 1.00 | 1.51 |
| GLU79 | HG3 | 1.00 | 0.019 | 1.00 | 1.51 |
| GLU79 | H | 1.00 | 0.004 | 1.00 | -2159032.00 |
| LEU80 | HA | 1.00 | 0.200 | 0.00 | 0.00 |
| LEU80 | H | 1.00 | 0.005 | 1.00 | -1212178.00 |

3.79.6 Detailed Probabilities of GLU79HB2:

Overall probability: 0.429

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU79 | 0.33 | 0.86 |
| LEU80 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E79HA | 1.00 |
| E79HB3 | 1.00 |
| E79HG2 | 1.00 |
| E79HG3 | 1.00 |
| E79H | 1.00 |
| E79HE2 | 1.00 |
| E79HB2 | 1.00 |
| L80H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU79 | HA | 1.00 | 0.012 | 1.00 | 2.52 |
| GLU79 | HB2 | 1.00 | 0.060 | 0.00 | 0.00 |
| GLU79 | HB3 | 1.00 | 0.054 | 0.00 | 0.00 |
| GLU79 | HG2 | 1.00 | 0.061 | 0.00 | 0.00 |
| GLU79 | HG3 | 1.00 | 0.061 | 0.00 | 0.00 |
| GLU79 | H | 1.00 | 0.005 | 1.00 | -1788928.00 |
| LEU80 | H | 1.00 | 0.000 | 1.00 | -719066.00 |

3.79.7 Detailed Probabilities of GLU79HB3:

Overall probability: 0.875

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU79 | 0.83 | 0.86 |
| LEU80 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E79HA | 1.00 |
| E79HB2 | 1.00 |
| E79HG2 | 1.00 |
| E79HG3 | 1.00 |
| E79H | 1.00 |
| E79HE2 | 1.00 |
| E79HB3 | 1.00 |
| L80H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU79 | HA | 1.00 | 0.063 | 0.00 | 0.00 |
| GLU79 | HB2 | 1.00 | 0.015 | 1.00 | 18.54 |
| GLU79 | HB3 | 1.00 | 0.021 | 1.00 | 18.77 |
| GLU79 | HG2 | 1.00 | 0.012 | 1.00 | 3.05 |
| GLU79 | HG3 | 1.00 | 0.012 | 1.00 | 3.05 |
| GLU79 | H | 1.00 | 0.009 | 1.00 | -2408894.00 |
| LEU80 | H | 1.00 | 0.009 | 1.00 | -932733.00 |
| LEU80 | HA | 0.87 | 0.002 | 1.00 | 0.07 |

3.79.8 Detailed Probabilities of GLU79HG2:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU79 | 1.00 | 0.86 |
| LEU80 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E79HA | 1.00 |
| E79HB2 | 1.00 |
| E79HB3 | 1.00 |
| E79HG3 | 1.00 |
| E79H | 1.00 |
| E79HE2 | 1.00 |
| E79HG2 | 1.00 |
| L80H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU79 | HA | 1.00 | 0.000 | 1.00 | 2.15 |
| GLU79 | HB2 | 1.00 | 0.011 | 1.00 | 2.72 |
| GLU79 | HB3 | 1.00 | 0.008 | 1.00 | 2.87 |
| GLU79 | HG2 | 1.00 | 0.010 | 1.00 | 180.23 |
| GLU79 | HG3 | 1.00 | 0.010 | 1.00 | 180.23 |
| GLU79 | H | 1.00 | 0.004 | 1.00 | -1654494.00 |
| LEU80 | H | 0.97 | 0.005 | 1.00 | -514014.00 |

3.79.9 Detailed Probabilities of GLU79HG3:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU79 | 1.00 | 0.86 |
| LEU80 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E79HA | 1.00 |
| E79HB2 | 1.00 |
| E79HB3 | 1.00 |
| E79HG2 | 1.00 |
| E79H | 1.00 |
| E79HE2 | 1.00 |
| E79HG3 | 1.00 |
| L80H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU79 | HA | 1.00 | 0.000 | 1.00 | 2.15 |
| GLU79 | HB2 | 1.00 | 0.011 | 1.00 | 2.72 |
| GLU79 | HB3 | 1.00 | 0.008 | 1.00 | 2.87 |
| GLU79 | HG2 | 1.00 | 0.010 | 1.00 | 180.23 |
| GLU79 | HG3 | 1.00 | 0.010 | 1.00 | 180.23 |
| GLU79 | H | 1.00 | 0.004 | 1.00 | -1654494.00 |
| LEU80 | H | 0.97 | 0.005 | 1.00 | -514014.00 |

3.79.10 Detailed Probabilities of GLU79H:

Overall probability: 0.857

Overall confidence: 0.923

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU78 | 0.80 | 0.83 |
| GLU79 | 0.83 | 1.00 |
| LEU80 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E78HG2 | 0.98 |
| E78HA | 1.00 |
| E78H | 1.00 |
| E78HB3 | 1.00 |
| E78HG3 | 0.97 |
| E78HB2 | 1.00 |
| E79HA | 1.00 |
| E79HB2 | 1.00 |
| E79HB3 | 1.00 |
| E79HG2 | 1.00 |
| E79HG3 | 1.00 |
| E79H | 1.00 |
| L80H | 1.00 |

NOESY contacts detailed probability

3.79 GLU(79)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU78 | HA | 1.00 | 0.114 | 0.00 | 0.00 |
| GLU78 | HB2 | 1.00 | 0.004 | 1.00 | 0.38 |
| GLU78 | HB3 | 1.00 | 0.004 | 1.00 | 0.38 |
| GLU78 | HG2 | 0.98 | 0.030 | 1.00 | 0.00 |
| GLU78 | HG3 | 0.97 | 0.030 | 1.00 | 0.00 |
| GLU79 | HA | 1.00 | 0.003 | 1.00 | 1.47 |
| GLU79 | HB2 | 1.00 | 0.008 | 1.00 | 0.73 |
| GLU79 | HB3 | 1.00 | 0.112 | 0.00 | 0.00 |
| GLU79 | HG2 | 1.00 | 0.008 | 1.00 | 0.77 |
| GLU79 | HG3 | 1.00 | 0.008 | 1.00 | 0.77 |
| GLU79 | H | 1.00 | 0.003 | 1.00 | -15771137.00 |
| LEU80 | H | 1.00 | 0.004 | 1.00 | -2684479.00 |
| LEU80 | HA | 0.93 | 0.011 | 1.00 | 0.08 |
| LEU80 | HB2 | 0.69 | 0.010 | 1.00 | 0.11 |

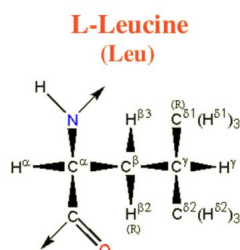
3.80 LEU(80)

Figure 70: Image from the BMRB

Residue probability: 0.766

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 175.080 | 177.056 | 1.929 | 0.000 | 0.000 |
| CA 3.80.1 | 54.138 | 55.735 | 3.802 | 0.750 | 1.000 |
| CB 3.80.2 | 42.541 | 42.389 | 3.750 | 0.875 | 1.000 |
| CG 3.80.3 | 26.770 | 26.892 | 3.086 | 0.625 | 1.000 |
| CD1 3.80.4 | 25.912 | 24.837 | 3.657 | 0.333 | 1.000 |
| CD2 3.80.5 | 24.730 | 24.201 | 3.117 | 0.857 | 1.000 |
| N 3.80.6 | 120.646 | 121.785 | 4.943 | 1.000 | 1.000 |
| HA 3.80.7 | 4.205 | 4.315 | 0.840 | 0.818 | 1.000 |
| HB2 3.80.8 | 1.418 | 1.601 | 0.373 | 0.750 | 1.000 |
| HB3 3.80.9 | 1.295 | 1.508 | 0.398 | 0.875 | 1.000 |
| HG 3.80.10 | 1.505 | 1.510 | 0.340 | 0.500 | 1.000 |
| HD1 3.80.11 | 0.953 | 0.739 | 0.294 | 0.857 | 1.000 |
| HD2 3.80.12 | 0.876 | 0.727 | 0.421 | 0.714 | 1.000 |
| H 3.80.13 | 7.042 | 8.237 | 0.647 | 1.000 | 1.000 |

3.80.1 Detailed Probabilities of LEU80CA:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU79 | 0.67 | 1.00 |
| LEU80 | 0.86 | 1.00 |
| ASP81 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E79HA | 1.00 |
| L80HB2 | 1.00 |
| L80HB3 | 1.00 |
| L80HG | 1.00 |
| L80HD11 | 0.99 |
| L80HD21 | 0.99 |
| L80H | 1.00 |
| L80HA | 1.00 |
| D81HA | 1.00 |
| D81H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU79 | HA | 1.00 | 0.200 | 0.00 | 0.00 |
| GLU79 | HB3 | 0.87 | 0.002 | 1.00 | 0.07 |
| GLU79 | H | 0.93 | 0.011 | 1.00 | 0.08 |
| LEU80 | HA | 1.00 | 0.002 | 1.00 | 7.95 |
| LEU80 | HB2 | 1.00 | 0.003 | 1.00 | 0.87 |
| LEU80 | HB3 | 1.00 | 0.003 | 1.00 | 0.79 |
| LEU80 | HG | 1.00 | 0.084 | 0.00 | 0.00 |
| LEU80 | HD11 | 0.99 | 0.004 | 1.00 | 0.55 |
| LEU80 | HD21 | 0.99 | 0.000 | 1.00 | 0.84 |
| LEU80 | H | 1.00 | 0.002 | 1.00 | 0.65 |
| ASP81 | HA | 1.00 | 0.214 | 0.00 | 0.00 |
| ASP81 | H | 1.00 | 0.003 | 1.00 | 1.91 |

3.80.2 Detailed Probabilities of LEU80CB:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU80 | 0.86 | 1.00 |
| ASP81 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L80HA | 1.00 |
| L80HB3 | 1.00 |
| L80HG | 1.00 |
| L80HD11 | 1.00 |
| L80HD21 | 1.00 |
| L80H | 1.00 |
| L80HB2 | 1.00 |
| D81H | 1.00 |

NOESY contacts detailed probability

3.80 LEU(80)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU80 | HA | 1.00 | 0.003 | 1.00 | 0.82 |
| LEU80 | HB2 | 1.00 | 0.002 | 1.00 | 6.87 |
| LEU80 | HB3 | 1.00 | 0.002 | 1.00 | 4.18 |
| LEU80 | HG | 1.00 | 0.089 | 0.00 | 0.00 |
| LEU80 | HD11 | 1.00 | 0.007 | 1.00 | 0.78 |
| LEU80 | HD21 | 1.00 | 0.003 | 1.00 | 0.79 |
| LEU80 | H | 1.00 | 0.002 | 1.00 | 1.27 |
| ASP81 | H | 1.00 | 0.005 | 1.00 | 0.20 |

3.80.3 Detailed Probabilities of LEU80CG:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU80 | 0.57 | 1.00 |
| ASP81 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L80HA | 1.00 |
| L80HB2 | 1.00 |
| L80HB3 | 1.00 |
| L80HD11 | 1.00 |
| L80HD21 | 1.00 |
| L80H | 1.00 |
| L80HG | 1.00 |
| D81H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU80 | HA | 1.00 | 0.064 | 0.00 | 0.00 |
| LEU80 | HB2 | 1.00 | 0.091 | 0.00 | 0.00 |
| LEU80 | HB3 | 1.00 | 0.003 | 1.00 | 0.90 |
| LEU80 | HG | 1.00 | 0.004 | 1.00 | 14.72 |
| LEU80 | HD11 | 1.00 | 0.003 | 1.00 | 1.50 |
| LEU80 | HD21 | 1.00 | 0.074 | 0.00 | 0.00 |
| LEU80 | H | 1.00 | 0.003 | 1.00 | 0.63 |
| ASP81 | H | 0.97 | 0.008 | 1.00 | 0.13 |

3.80.4 Detailed Probabilities of LEU80CD1:

Overall probability: 0.333

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU80 | 0.33 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L80HA | 0.99 |
| L80HB2 | 1.00 |
| L80HB3 | 1.00 |
| L80HG | 1.00 |
| L80HD12 | 1.00 |
| L80HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU80 | HA | 0.99 | 0.001 | 1.00 | 0.53 |
| LEU80 | HB2 | 1.00 | 0.095 | 0.00 | 0.00 |
| LEU80 | HB3 | 1.00 | 0.132 | 0.00 | 0.00 |
| LEU80 | HG | 1.00 | 0.008 | 1.00 | 2.02 |
| LEU80 | HD11 | 1.00 | 0.199 | 0.00 | 0.00 |
| LEU80 | HD21 | 1.00 | 0.122 | 0.00 | 0.00 |

3.80.5 Detailed Probabilities of LEU80CD2:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU80 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L80HA | 0.99 |
| L80HB2 | 1.00 |
| L80HB3 | 1.00 |
| L80HG | 1.00 |
| L80HD11 | 1.00 |
| L80HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU80 | HA | 0.99 | 0.003 | 1.00 | 1.22 |
| LEU80 | HB2 | 1.00 | 0.026 | 1.00 | 3.10 |
| LEU80 | HB3 | 1.00 | 0.000 | 1.00 | 2.06 |
| LEU80 | HG | 1.00 | 0.061 | 0.00 | 0.00 |
| LEU80 | HD11 | 1.00 | 0.011 | 1.00 | 5.99 |
| LEU80 | HD21 | 1.00 | 0.012 | 1.00 | 205.58 |
| LEU80 | H | 0.85 | 0.006 | 1.00 | 0.50 |

3.80.6 Detailed Probabilities of LEU80N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU79 | 1.00 | 1.00 |
| LEU80 | 1.00 | 1.00 |
| ASP81 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E79HB2 | 1.00 |
| E79HG2 | 0.98 |
| E79HG3 | 0.97 |
| E79HB3 | 1.00 |
| E79H | 1.00 |
| E79HA | 1.00 |
| L80HA | 1.00 |
| L80HB2 | 1.00 |
| L80HB3 | 1.00 |
| L80HG | 1.00 |
| L80H | 1.00 |
| D81H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU79 | HA | 1.00 | 0.005 | 1.00 | -1212178.00 |
| GLU79 | HB2 | 1.00 | 0.000 | 1.00 | -719066.00 |
| GLU79 | HB3 | 1.00 | 0.009 | 1.00 | -932733.00 |
| GLU79 | HG2 | 0.98 | 0.004 | 1.00 | -514014.00 |
| GLU79 | HG3 | 0.97 | 0.005 | 1.00 | -514014.00 |
| GLU79 | H | 1.00 | 0.004 | 1.00 | -2684479.00 |
| LEU80 | HA | 1.00 | 0.004 | 1.00 | -1553284.00 |
| LEU80 | HB2 | 1.00 | 0.003 | 1.00 | -2773897.00 |
| LEU80 | HB3 | 1.00 | 0.002 | 1.00 | -2085034.00 |
| LEU80 | HG | 1.00 | 0.004 | 1.00 | -1476437.00 |
| LEU80 | H | 1.00 | 0.001 | 1.00 | -24148076.00 |
| LEU80 | HD11 | 0.88 | 0.005 | 1.00 | -536759.00 |
| LEU80 | HD21 | 0.87 | 0.007 | 1.00 | -647174.00 |
| ASP81 | H | 1.00 | 0.007 | 1.00 | -379272.00 |

3.80.7 Detailed Probabilities of LEU80HA:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU79 | 1.00 | 1.00 |
| LEU80 | 0.86 | 1.00 |
| ASP81 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E79HA | 1.00 |
| L80HB2 | 1.00 |
| L80HB3 | 1.00 |
| L80HG | 1.00 |
| L80HD11 | 0.99 |
| L80HD21 | 0.99 |
| L80H | 1.00 |
| L80HA | 1.00 |
| D81HA | 1.00 |
| D81H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU79 | HA | 1.00 | 0.004 | 1.00 | 0.23 |
| GLU79 | H | 0.93 | 0.007 | 1.00 | -180036.00 |
| LEU80 | HA | 1.00 | 0.002 | 1.00 | 7.95 |
| LEU80 | HB2 | 1.00 | 0.003 | 1.00 | 0.82 |
| LEU80 | HB3 | 1.00 | 0.004 | 1.00 | 0.87 |
| LEU80 | HG | 1.00 | 0.064 | 0.00 | 0.00 |
| LEU80 | HD11 | 0.99 | 0.001 | 1.00 | 0.53 |
| LEU80 | HD21 | 0.99 | 0.003 | 1.00 | 1.22 |
| LEU80 | H | 1.00 | 0.004 | 1.00 | -1553284.00 |
| ASP81 | HA | 1.00 | 0.287 | 0.00 | 0.00 |
| ASP81 | H | 1.00 | 0.004 | 1.00 | -4759384.00 |

3.80.8 Detailed Probabilities of LEU80HB2:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU80 | 0.71 | 1.00 |
| ASP81 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L80HA | 1.00 |
| L80HB3 | 1.00 |
| L80HG | 1.00 |
| L80HD11 | 1.00 |
| L80HD21 | 1.00 |
| L80H | 1.00 |
| L80HB2 | 1.00 |
| D81H | 1.00 |

NOESY contacts detailed probability

3.80 LEU(80)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU80 | HA | 1.00 | 0.003 | 1.00 | 0.87 |
| LEU80 | HB2 | 1.00 | 0.002 | 1.00 | 6.87 |
| LEU80 | HB3 | 1.00 | 0.003 | 1.00 | 4.42 |
| LEU80 | HG | 1.00 | 0.091 | 0.00 | 0.00 |
| LEU80 | HD11 | 1.00 | 0.095 | 0.00 | 0.00 |
| LEU80 | HD21 | 1.00 | 0.026 | 1.00 | 3.10 |
| LEU80 | H | 1.00 | 0.003 | 1.00 | -2773897.00 |
| ASP81 | H | 1.00 | 0.002 | 1.00 | -399434.00 |

3.80.9 Detailed Probabilities of LEU80HB3:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU80 | 0.86 | 1.00 |
| ASP81 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L80HA | 1.00 |
| L80HB2 | 1.00 |
| L80HG | 1.00 |
| L80HD11 | 1.00 |
| L80HD21 | 1.00 |
| L80H | 1.00 |
| L80HB3 | 1.00 |
| D81H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU80 | HA | 1.00 | 0.003 | 1.00 | 0.79 |
| LEU80 | HB2 | 1.00 | 0.002 | 1.00 | 4.18 |
| LEU80 | HB3 | 1.00 | 0.002 | 1.00 | 6.76 |
| LEU80 | HG | 1.00 | 0.003 | 1.00 | 0.90 |
| LEU80 | HD11 | 1.00 | 0.132 | 0.00 | 0.00 |
| LEU80 | HD21 | 1.00 | 0.000 | 1.00 | 2.06 |
| LEU80 | H | 1.00 | 0.002 | 1.00 | -2085034.00 |
| ASP81 | H | 1.00 | 0.003 | 1.00 | -586175.00 |

3.80.10 Detailed Probabilities of LEU80HG:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU80 | 0.43 | 1.00 |
| ASP81 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L80HA | 1.00 |
| L80HB2 | 1.00 |
| L80HB3 | 1.00 |
| L80HD11 | 1.00 |
| L80HD21 | 1.00 |
| L80H | 1.00 |
| L80HG | 1.00 |
| D81H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU80 | HA | 1.00 | 0.084 | 0.00 | 0.00 |
| LEU80 | HB2 | 1.00 | 0.089 | 0.00 | 0.00 |
| LEU80 | HB3 | 1.00 | 0.090 | 0.00 | 0.00 |
| LEU80 | HG | 1.00 | 0.004 | 1.00 | 14.72 |
| LEU80 | HD11 | 1.00 | 0.008 | 1.00 | 2.02 |
| LEU80 | HD21 | 1.00 | 0.061 | 0.00 | 0.00 |
| LEU80 | H | 1.00 | 0.004 | 1.00 | -1476437.00 |
| ASP81 | H | 0.97 | 0.006 | 1.00 | -290039.00 |

3.80.11 Detailed Probabilities of LEU80HD11:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU80 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L80HA | 0.99 |
| L80HB2 | 1.00 |
| L80HB3 | 1.00 |
| L80HG | 1.00 |
| L80HD12 | 1.00 |
| L80HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU80 | HA | 0.99 | 0.004 | 1.00 | 0.55 |
| LEU80 | HB2 | 1.00 | 0.007 | 1.00 | 0.78 |
| LEU80 | HB3 | 1.00 | 0.012 | 1.00 | 0.69 |
| LEU80 | HG | 1.00 | 0.003 | 1.00 | 1.50 |
| LEU80 | HD11 | 1.00 | 0.199 | 0.00 | 0.00 |
| LEU80 | HD21 | 1.00 | 0.011 | 1.00 | 5.99 |
| LEU80 | H | 0.86 | 0.005 | 1.00 | -536759.00 |

3.80.12 Detailed Probabilities of LEU80HD21:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU80 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L80HA | 0.99 |
| L80HB2 | 1.00 |
| L80HB3 | 1.00 |
| L80HG | 1.00 |
| L80HD11 | 1.00 |
| L80HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU80 | HA | 0.99 | 0.000 | 1.00 | 0.84 |
| LEU80 | HB2 | 1.00 | 0.003 | 1.00 | 0.79 |
| LEU80 | HB3 | 1.00 | 0.003 | 1.00 | 0.93 |
| LEU80 | HG | 1.00 | 0.074 | 0.00 | 0.00 |
| LEU80 | HD11 | 1.00 | 0.122 | 0.00 | 0.00 |
| LEU80 | HD21 | 1.00 | 0.012 | 1.00 | 205.58 |
| LEU80 | H | 0.85 | 0.007 | 1.00 | -647174.00 |

3.80.13 Detailed Probabilities of LEU80H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU79 | 1.00 | 1.00 |
| LEU80 | 1.00 | 1.00 |
| ASP81 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| E79HB2 | 1.00 |
| E79HG2 | 0.98 |
| E79HG3 | 0.97 |
| E79HB3 | 1.00 |
| E79H | 1.00 |
| E79HA | 1.00 |
| L80HA | 1.00 |
| L80HB2 | 1.00 |
| L80HB3 | 1.00 |
| L80HG | 1.00 |
| L80H | 1.00 |
| D81H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU79 | HA | 1.00 | 0.026 | 1.00 | 0.64 |
| GLU79 | HB2 | 1.00 | 0.000 | 1.00 | 0.26 |
| GLU79 | HB3 | 1.00 | 0.001 | 1.00 | 0.29 |
| GLU79 | HG2 | 0.98 | 0.017 | 1.00 | 0.17 |
| GLU79 | HG3 | 0.97 | 0.017 | 1.00 | 0.17 |
| GLU79 | H | 1.00 | 0.000 | 1.00 | -2754307.00 |
| LEU80 | HA | 1.00 | 0.002 | 1.00 | 0.65 |
| LEU80 | HB2 | 1.00 | 0.002 | 1.00 | 1.27 |
| LEU80 | HB3 | 1.00 | 0.001 | 1.00 | 1.12 |
| LEU80 | HG | 1.00 | 0.003 | 1.00 | 0.63 |
| LEU80 | H | 1.00 | 0.001 | 1.00 | -24148076.00 |
| LEU80 | HD21 | 0.87 | 0.006 | 1.00 | 0.50 |
| ASP81 | H | 1.00 | 0.002 | 1.00 | -356427.00 |
| ASP81 | HA | 0.90 | 0.020 | 1.00 | 0.12 |

3.81 ASP(81)

Figure 71: Image from the BMRB

Residue probability: 0.873

Residue probability confidence: 0.893

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 178.227 | 176.463 | 2.348 | 0.000 | 0.000 |
| CA 3.81.1 | 53.559 | 54.786 | 4.266 | 0.750 | 0.875 |
| CB 3.81.2 | 42.676 | 40.949 | 3.070 | 1.000 | 0.833 |
| N 3.81.3 | 126.651 | 120.550 | 5.690 | 1.000 | 1.000 |
| HD2 | NA | – | – | 0.000 | 0.000 |
| HA 3.81.4 | 4.567 | 4.587 | 0.329 | 0.814 | 0.875 |
| HB2 3.81.5 | 2.833 | 2.708 | 0.282 | 0.833 | 0.833 |
| HB3 3.81.6 | 2.704 | 2.654 | 0.285 | 0.800 | 0.833 |
| H 3.81.7 | 8.479 | 8.304 | 1.027 | 0.917 | 1.000 |

3.81.1 Detailed Probabilities of ASP81CA:

Overall probability: 0.750

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU80 | 0.50 | 1.00 |
| ASP81 | 0.75 | 0.80 |
| TRP82 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L80HA | 1.00 |
| D81HD2 | 1.00 |
| D81HB2 | 1.00 |
| D81HB3 | 1.00 |
| D81H | 1.00 |
| D81HA | 1.00 |
| W82H | 1.00 |
| W82HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU80 | HA | 1.00 | 0.287 | 0.00 | 0.00 |
| LEU80 | H | 0.90 | 0.020 | 1.00 | 0.12 |
| ASP81 | HA | 1.00 | 0.005 | 1.00 | 6.40 |
| ASP81 | HB2 | 1.00 | 0.003 | 1.00 | 0.75 |
| ASP81 | HB3 | 1.00 | 0.009 | 1.00 | 1.07 |
| ASP81 | H | 1.00 | 0.113 | 0.00 | 0.00 |
| TRP82 | HA | 1.00 | 0.025 | 1.00 | 6.40 |
| TRP82 | H | 1.00 | 0.005 | 1.00 | 1.03 |

3.81.2 Detailed Probabilities of ASP81CB:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP81 | 1.00 | 0.80 |
| TRP82 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D81HD2 | 1.00 |
| D81HA | 1.00 |
| D81HB2 | 1.00 |
| D81H | 1.00 |
| D81HB3 | 1.00 |
| W82H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP81 | HA | 1.00 | 0.004 | 1.00 | 0.60 |
| ASP81 | HB2 | 1.00 | 0.000 | 1.00 | 3.53 |
| ASP81 | HB3 | 1.00 | 0.001 | 1.00 | 3.88 |
| ASP81 | H | 1.00 | 0.004 | 1.00 | 0.85 |
| TRP82 | H | 1.00 | 0.003 | 1.00 | 0.08 |
| TRP82 | HA | 0.86 | 0.026 | 1.00 | 0.60 |

3.81.3 Detailed Probabilities of ASP81N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU80 | 1.00 | 1.00 |
| ASP81 | 1.00 | 1.00 |
| TRP82 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L80H | 1.00 |
| L80HB2 | 1.00 |
| L80HB3 | 1.00 |
| L80HA | 1.00 |
| L80HG | 0.97 |
| D81HA | 1.00 |
| D81HB2 | 1.00 |
| D81HB3 | 1.00 |
| D81H | 1.00 |
| W82H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU80 | HA | 1.00 | 0.004 | 1.00 | -4759384.00 |
| LEU80 | HB2 | 1.00 | 0.002 | 1.00 | -399434.00 |
| LEU80 | HB3 | 1.00 | 0.003 | 1.00 | -586175.00 |
| LEU80 | HG | 0.97 | 0.006 | 1.00 | -290039.00 |
| LEU80 | H | 1.00 | 0.002 | 1.00 | -356427.00 |
| LEU80 | HD11 | 0.54 | 0.021 | 1.00 | -631482.00 |
| ASP81 | HA | 1.00 | 0.004 | 1.00 | -861915.00 |
| ASP81 | HB2 | 1.00 | 0.002 | 1.00 | -2082316.00 |
| ASP81 | HB3 | 1.00 | 0.001 | 1.00 | -2072140.00 |
| ASP81 | H | 1.00 | 0.003 | 1.00 | -10551273.00 |
| TRP82 | H | 1.00 | 0.006 | 1.00 | -105645.00 |
| TRP82 | HA | 0.90 | 0.026 | 1.00 | -861915.00 |

3.81.4 Detailed Probabilities of ASP81HA:

Overall probability: 0.814

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU80 | 0.00 | 1.00 |
| ASP81 | 1.00 | 0.80 |
| TRP82 | 0.85 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L80HA | 1.00 |
| D81HD2 | 1.00 |
| D81HB2 | 1.00 |
| D81HB3 | 1.00 |
| D81H | 1.00 |
| D81HA | 1.00 |
| W82H | 1.00 |
| W82HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU80 | HA | 1.00 | 0.214 | 0.00 | 0.00 |
| ASP81 | HA | 1.00 | 0.005 | 1.00 | 6.40 |
| ASP81 | HB2 | 1.00 | 0.003 | 1.00 | 0.44 |
| ASP81 | HB3 | 1.00 | 0.004 | 1.00 | 0.60 |
| ASP81 | H | 1.00 | 0.004 | 1.00 | -861915.00 |
| TRP82 | HA | 1.00 | 0.033 | 0.70 | 0.00 |
| TRP82 | H | 1.00 | 0.008 | 1.00 | -1801510.00 |

3.81.5 Detailed Probabilities of ASP81HB2:

Overall probability: 0.833

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP81 | 0.75 | 0.80 |
| TRP82 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D81HD2 | 1.00 |
| D81HA | 1.00 |
| D81HB3 | 1.00 |
| D81H | 1.00 |
| D81HB2 | 1.00 |
| W82H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP81 | HA | 1.00 | 0.003 | 1.00 | 0.75 |
| ASP81 | HB2 | 1.00 | 0.898 | 0.00 | 0.00 |
| ASP81 | HB3 | 1.00 | 0.000 | 1.00 | 3.53 |
| ASP81 | H | 1.00 | 0.002 | 1.00 | -2082316.00 |
| TRP82 | H | 1.00 | 0.003 | 1.00 | -149287.00 |
| TRP82 | HA | 0.61 | 0.022 | 1.00 | 0.06 |

3.81.6 Detailed Probabilities of ASP81HB3:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP81 | 0.75 | 0.80 |
| TRP82 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D81HD2 | 1.00 |
| D81HA | 1.00 |
| D81HB2 | 1.00 |
| D81H | 1.00 |
| D81HB3 | 1.00 |
| W82H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP81 | HA | 1.00 | 0.009 | 1.00 | 1.07 |
| ASP81 | HB2 | 1.00 | 0.769 | 0.00 | 0.00 |
| ASP81 | HB3 | 1.00 | 0.001 | 1.00 | 3.88 |
| ASP81 | H | 1.00 | 0.001 | 1.00 | -2072140.00 |
| TRP82 | H | 1.00 | 0.007 | 1.00 | -209973.00 |

3.81.7 Detailed Probabilities of ASP81H:

Overall probability: 0.917

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU80 | 1.00 | 1.00 |
| ASP81 | 0.75 | 1.00 |
| TRP82 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L80H | 1.00 |
| L80HB2 | 1.00 |
| L80HB3 | 1.00 |
| L80HA | 1.00 |
| L80HG | 0.97 |
| D81HA | 1.00 |
| D81HB2 | 1.00 |
| D81HB3 | 1.00 |
| D81H | 1.00 |
| W82H | 1.00 |

NOESY contacts detailed probability

3.81 ASP(81)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU80 | HA | 1.00 | 0.003 | 1.00 | 1.91 |
| LEU80 | HB2 | 1.00 | 0.005 | 1.00 | 0.20 |
| LEU80 | HB3 | 1.00 | 0.003 | 1.00 | 0.27 |
| LEU80 | HG | 0.97 | 0.008 | 1.00 | 0.13 |
| LEU80 | H | 1.00 | 0.007 | 1.00 | -379272.00 |
| LEU80 | HD11 | 0.54 | 0.004 | 1.00 | 0.31 |
| LEU80 | HD21 | 0.58 | 0.003 | 1.00 | 0.42 |
| ASP81 | HA | 1.00 | 0.113 | 0.00 | 0.00 |
| ASP81 | HB2 | 1.00 | 0.004 | 1.00 | 0.77 |
| ASP81 | HB3 | 1.00 | 0.004 | 1.00 | 0.85 |
| ASP81 | H | 1.00 | 0.003 | 1.00 | -10551273.00 |
| TRP82 | H | 1.00 | 0.006 | 1.00 | -109396.00 |

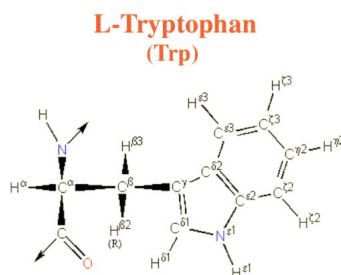
3.82 TRP(82)

Figure 72: Image from the BMRB

Residue probability: 0.823

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 179.215 | 176.178 | 2.019 | 0.000 | 0.000 |
| CA 3.82.1 | 60.626 | 57.713 | 2.717 | 0.736 | 1.000 |
| CB 3.82.2 | 30.438 | 30.144 | 3.081 | 0.778 | 1.000 |
| CD1 3.82.3 | 127.686 | 126.068 | 7.070 | 0.875 | 1.000 |
| CE3 3.82.4 | 120.380 | 120.123 | 5.387 | 0.556 | 1.000 |
| CZ2 3.82.5 | 115.636 | 114.015 | 4.831 | 1.000 | 1.000 |
| CZ3 3.82.6 | 120.286 | 121.013 | 5.400 | 0.500 | 1.000 |
| CH2 3.82.7 | 124.501 | 123.568 | 4.896 | 0.800 | 1.000 |
| N 3.82.8 | 126.943 | 121.531 | 4.451 | 1.000 | 1.000 |
| NE1 3.82.9 | 127.196 | 129.267 | 3.325 | 1.000 | 1.000 |
| HA 3.82.10 | 4.597 | 4.675 | 0.550 | 0.985 | 1.000 |
| HB2 3.82.11 | 3.343 | 3.173 | 0.355 | 0.889 | 1.000 |
| HB3 3.82.12 | 3.195 | 3.093 | 0.388 | 1.000 | 1.000 |
| HD1 3.82.13 | 7.534 | 7.154 | 2.084 | 0.750 | 1.000 |
| HE3 3.82.14 | 7.658 | 7.268 | 0.457 | 0.889 | 1.000 |
| HZ2 3.82.15 | 7.353 | 7.261 | 0.347 | 0.667 | 1.000 |
| HZ3 3.82.16 | 6.829 | 6.836 | 0.396 | 0.750 | 1.000 |
| HH2 3.82.17 | 7.191 | 6.945 | 0.376 | 1.000 | 1.000 |
| H 3.82.18 | 9.372 | 8.314 | 1.088 | 0.970 | 1.000 |
| HE1 3.82.19 | 9.809 | 10.060 | 0.770 | 0.500 | 1.000 |

3.82.1 Detailed Probabilities of TRP82CA:

Overall probability: 0.736

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP81 | 0.85 | 1.00 |
| TRP82 | 0.81 | 1.00 |
| ASN83 | 0.35 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D81HA | 1.00 |
| W82HB2 | 1.00 |
| W82HB3 | 1.00 |
| W82HD1 | 1.00 |
| W82HE3 | 1.00 |
| W82H | 1.00 |
| W82HA | 1.00 |
| N83H | 1.00 |
| N83HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP81 | HA | 1.00 | 0.033 | 0.70 | 0.00 |
| ASP81 | HB2 | 0.61 | 0.022 | 1.00 | 0.06 |
| TRP82 | HA | 1.00 | 0.003 | 1.00 | 5.11 |
| TRP82 | HB2 | 1.00 | 0.008 | 1.00 | 0.30 |
| TRP82 | HB3 | 1.00 | 0.007 | 1.00 | 0.55 |
| TRP82 | HD1 | 1.00 | 0.087 | 0.00 | 0.00 |
| TRP82 | HE3 | 1.00 | 0.003 | 1.00 | 1.02 |
| TRP82 | H | 1.00 | 0.033 | 0.70 | 0.00 |
| TRP82 | HE1 | 0.60 | 0.023 | 1.00 | 0.16 |
| ASN83 | HA | 1.00 | 0.033 | 0.70 | 0.00 |
| ASN83 | H | 1.00 | 0.171 | 0.00 | 0.00 |

3.82.2 Detailed Probabilities of TRP82CB:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 0.86 | 1.00 |
| ASN83 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| W82HA | 1.00 |
| W82HB3 | 1.00 |
| W82HD1 | 1.00 |
| W82HE3 | 1.00 |
| W82H | 1.00 |
| W82HE1 | 1.00 |
| W82HB2 | 1.00 |
| N83H | 1.00 |

NOESY contacts detailed probability

3.82 TRP(82)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HA | 1.00 | 0.006 | 1.00 | 0.32 |
| TRP82 | HB2 | 1.00 | 0.001 | 1.00 | 1.33 |
| TRP82 | HB3 | 1.00 | 0.003 | 1.00 | 1.32 |
| TRP82 | HD1 | 1.00 | 0.001 | 1.00 | 0.28 |
| TRP82 | HE3 | 1.00 | 0.003 | 1.00 | 0.14 |
| TRP82 | H | 1.00 | 0.002 | 1.00 | 0.18 |
| TRP82 | HE1 | 1.00 | 0.439 | 0.00 | 0.00 |
| ASN83 | H | 1.00 | 0.291 | 0.00 | 0.00 |
| ASN83 | HA | 0.63 | 0.024 | 1.00 | 0.32 |

3.82.3 Detailed Probabilities of TRP82CD1:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 0.88 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| W82HA | 1.00 |
| W82HB2 | 1.00 |
| W82HB3 | 1.00 |
| W82HE3 | 1.00 |
| W82HZ2 | 1.00 |
| W82H | 0.99 |
| W82HE1 | 1.00 |
| W82HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HA | 1.00 | 0.000 | 1.00 | 0.26 |
| TRP82 | HB2 | 1.00 | 0.001 | 1.00 | 0.23 |
| TRP82 | HB3 | 1.00 | 0.000 | 1.00 | 0.15 |
| TRP82 | HD1 | 1.00 | 0.001 | 1.00 | 4.39 |
| TRP82 | HE3 | 1.00 | 0.122 | 0.00 | 0.00 |
| TRP82 | HZ2 | 1.00 | 0.006 | 1.00 | 0.25 |
| TRP82 | H | 0.99 | 0.003 | 1.00 | 0.25 |
| TRP82 | HE1 | 1.00 | 0.004 | 1.00 | 0.62 |

3.82.4 Detailed Probabilities of TRP82CE3:

Overall probability: 0.556

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 0.56 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| W82HA | 1.00 |
| W82HB2 | 1.00 |
| W82HB3 | 1.00 |
| W82HD1 | 1.00 |
| W82HZ2 | 1.00 |
| W82HZ3 | 1.00 |
| W82HH2 | 1.00 |
| W82HE1 | 1.00 |
| W82HE3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HA | 1.00 | 0.005 | 1.00 | 0.26 |
| TRP82 | HB2 | 1.00 | 0.137 | 0.00 | 0.00 |
| TRP82 | HB3 | 1.00 | 0.011 | 1.00 | 0.07 |
| TRP82 | HD1 | 1.00 | 0.100 | 0.00 | 0.00 |
| TRP82 | HE3 | 1.00 | 0.000 | 1.00 | 1.69 |
| TRP82 | HZ2 | 1.00 | 0.081 | 0.00 | 0.00 |
| TRP82 | HZ3 | 1.00 | 0.000 | 1.00 | 0.27 |
| TRP82 | HH2 | 1.00 | 0.001 | 1.00 | 0.16 |
| TRP82 | HE1 | 1.00 | 1.147 | 0.00 | 0.00 |

3.82.5 Detailed Probabilities of TRP82CZ2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| W82HD1 | 1.00 |
| W82HE3 | 1.00 |
| W82HZ3 | 1.00 |
| W82HH2 | 1.00 |
| W82HE1 | 1.00 |
| W82HZ2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HD1 | 1.00 | 0.027 | 1.00 | 0.09 |
| TRP82 | HE3 | 1.00 | 0.009 | 1.00 | 0.09 |
| TRP82 | HZ2 | 1.00 | 0.006 | 1.00 | 6.41 |
| TRP82 | HZ3 | 1.00 | 0.000 | 1.00 | 0.20 |
| TRP82 | HH2 | 1.00 | 0.001 | 1.00 | 1.56 |
| TRP82 | HE1 | 1.00 | 0.002 | 1.00 | 0.20 |

3.82.6 Detailed Probabilities of TRP82CZ3:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| W82HE3 | 1.00 |
| W82HZ2 | 1.00 |
| W82HH2 | 1.00 |
| W82HZ3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HE3 | 1.00 | 0.007 | 1.00 | 0.99 |
| TRP82 | HZ2 | 1.00 | 0.167 | 0.00 | 0.00 |
| TRP82 | HZ3 | 1.00 | 0.154 | 0.00 | 0.00 |
| TRP82 | HH2 | 1.00 | 0.005 | 1.00 | 0.20 |

3.82.7 Detailed Probabilities of TRP82CH2:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 0.80 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| W82HE3 | 1.00 |
| W82HZ2 | 1.00 |
| W82HZ3 | 1.00 |
| W82HE1 | 1.00 |
| W82HH2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HE3 | 1.00 | 0.020 | 1.00 | 0.13 |
| TRP82 | HZ2 | 1.00 | 0.003 | 1.00 | 0.41 |
| TRP82 | HZ3 | 1.00 | 0.002 | 1.00 | 1.18 |
| TRP82 | HH2 | 1.00 | 0.004 | 1.00 | 6.58 |
| TRP82 | HE1 | 1.00 | 0.334 | 0.00 | 0.00 |

3.82.8 Detailed Probabilities of TRP82N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP81 | 1.00 | 1.00 |
| TRP82 | 1.00 | 1.00 |
| ASN83 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D81H | 1.00 |
| D81HB2 | 1.00 |
| D81HA | 1.00 |
| D81HB3 | 1.00 |
| W82HA | 1.00 |
| W82HB2 | 1.00 |
| W82HB3 | 1.00 |
| W82HD1 | 0.99 |
| W82H | 1.00 |
| N83H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP81 | HA | 1.00 | 0.008 | 1.00 | -1801510.00 |
| ASP81 | HB2 | 1.00 | 0.003 | 1.00 | -149287.00 |
| ASP81 | HB3 | 1.00 | 0.007 | 1.00 | -209973.00 |
| ASP81 | H | 1.00 | 0.006 | 1.00 | -109396.00 |
| TRP82 | HA | 1.00 | 0.022 | 1.00 | -1801510.00 |
| TRP82 | HB2 | 1.00 | 0.003 | 1.00 | -566343.00 |
| TRP82 | HB3 | 1.00 | 0.004 | 1.00 | -414942.00 |
| TRP82 | HD1 | 0.99 | 0.001 | 1.00 | -242133.00 |
| TRP82 | H | 1.00 | 0.006 | 1.00 | -2069368.00 |
| ASN83 | H | 1.00 | 0.002 | 1.00 | -122598.00 |
| ASN83 | HA | 0.85 | 0.008 | 1.00 | -1801510.00 |

3.82.9 Detailed Probabilities of TRP82NE1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| W82HB2 | 1.00 |
| W82HB3 | 1.00 |
| W82HD1 | 1.00 |
| W82HE3 | 1.00 |
| W82HZ2 | 1.00 |
| W82HH2 | 1.00 |
| W82HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HB2 | 1.00 | 0.000 | 1.00 | -96717.00 |
| TRP82 | HB3 | 1.00 | 0.010 | 1.00 | -140471.00 |
| TRP82 | HD1 | 1.00 | 0.000 | 1.00 | -2179132.00 |
| TRP82 | HE3 | 1.00 | 0.011 | 1.00 | -95024.00 |
| TRP82 | HZ2 | 1.00 | 0.008 | 1.00 | -871290.00 |
| TRP82 | HH2 | 1.00 | 0.000 | 1.00 | -146404.00 |
| TRP82 | HE1 | 1.00 | 0.003 | 1.00 | -10815338.00 |
| TRP82 | HA | 0.60 | 0.017 | 1.00 | -143085.00 |

3.82.10 Detailed Probabilities of TRP82HA:

Overall probability: 0.985

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP81 | 1.00 | 1.00 |
| TRP82 | 1.00 | 1.00 |
| ASN83 | 0.90 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D81HA | 1.00 |
| W82HB2 | 1.00 |
| W82HB3 | 1.00 |
| W82HD1 | 1.00 |
| W82HE3 | 1.00 |
| W82H | 1.00 |
| W82HA | 1.00 |
| N83H | 1.00 |
| N83HA | 1.00 |

NOESY contacts detailed probability

3.82 TRP(82)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP81 | HA | 1.00 | 0.025 | 1.00 | 6.40 |
| ASP81 | HB2 | 0.61 | 0.027 | 1.00 | 0.44 |
| ASP81 | HB3 | 0.86 | 0.026 | 1.00 | 0.60 |
| ASP81 | H | 0.90 | 0.026 | 1.00 | -861915.00 |
| TRP82 | HA | 1.00 | 0.003 | 1.00 | 5.11 |
| TRP82 | HB2 | 1.00 | 0.006 | 1.00 | 0.32 |
| TRP82 | HB3 | 1.00 | 0.001 | 1.00 | 0.40 |
| TRP82 | HD1 | 1.00 | 0.000 | 1.00 | 0.26 |
| TRP82 | HE3 | 1.00 | 0.005 | 1.00 | 0.26 |
| TRP82 | H | 1.00 | 0.022 | 1.00 | -1801510.00 |
| TRP82 | HE1 | 0.60 | 0.017 | 1.00 | -143085.00 |
| ASN83 | HA | 1.00 | 0.025 | 1.00 | 51.32 |
| ASN83 | H | 1.00 | 0.032 | 0.80 | 0.00 |

3.82.11 Detailed Probabilities of TRP82HB2:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 0.86 | 1.00 |
| ASN83 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| W82HA | 1.00 |
| W82HB3 | 1.00 |
| W82HD1 | 1.00 |
| W82HE3 | 1.00 |
| W82H | 1.00 |
| W82HE1 | 1.00 |
| W82HB2 | 1.00 |
| N83H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HA | 1.00 | 0.008 | 1.00 | 0.30 |
| TRP82 | HB2 | 1.00 | 0.001 | 1.00 | 1.33 |
| TRP82 | HB3 | 1.00 | 0.000 | 1.00 | 1.27 |
| TRP82 | HD1 | 1.00 | 0.001 | 1.00 | 0.23 |
| TRP82 | HE3 | 1.00 | 0.137 | 0.00 | 0.00 |
| TRP82 | H | 1.00 | 0.003 | 1.00 | -566343.00 |
| TRP82 | HE1 | 1.00 | 0.000 | 1.00 | -96717.00 |
| ASN83 | H | 1.00 | 0.001 | 1.00 | -141336.00 |
| ASN83 | HA | 0.63 | 0.004 | 1.00 | 0.06 |

3.82.12 Detailed Probabilities of TRP82HB3:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 1.00 | 1.00 |
| ASN83 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| W82HA | 1.00 |
| W82HB2 | 1.00 |
| W82HD1 | 1.00 |
| W82HE3 | 1.00 |
| W82H | 1.00 |
| W82HE1 | 1.00 |
| W82HB3 | 1.00 |
| N83H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HA | 1.00 | 0.007 | 1.00 | 0.55 |
| TRP82 | HB2 | 1.00 | 0.003 | 1.00 | 1.32 |
| TRP82 | HB3 | 1.00 | 0.003 | 1.00 | 1.53 |
| TRP82 | HD1 | 1.00 | 0.000 | 1.00 | 0.15 |
| TRP82 | HE3 | 1.00 | 0.011 | 1.00 | 0.07 |
| TRP82 | H | 1.00 | 0.004 | 1.00 | -414942.00 |
| TRP82 | HE1 | 1.00 | 0.010 | 1.00 | -140471.00 |
| ASN83 | H | 1.00 | 0.005 | 1.00 | -96149.00 |
| ASN83 | HA | 0.81 | 0.025 | 1.00 | 0.14 |

3.82.13 Detailed Probabilities of TRP82HD1:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 0.75 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| W82HA | 1.00 |
| W82HB2 | 1.00 |
| W82HB3 | 1.00 |
| W82HE3 | 1.00 |
| W82HZ2 | 1.00 |
| W82H | 0.99 |
| W82HE1 | 1.00 |
| W82HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HA | 1.00 | 0.087 | 0.00 | 0.00 |
| TRP82 | HB2 | 1.00 | 0.001 | 1.00 | 0.28 |
| TRP82 | HB3 | 1.00 | 0.002 | 1.00 | 0.20 |
| TRP82 | HD1 | 1.00 | 0.001 | 1.00 | 4.39 |
| TRP82 | HE3 | 1.00 | 0.100 | 0.00 | 0.00 |
| TRP82 | HZ2 | 1.00 | 0.027 | 1.00 | 0.09 |
| TRP82 | H | 0.99 | 0.001 | 1.00 | -242133.00 |
| TRP82 | HE1 | 1.00 | 0.000 | 1.00 | -2179132.00 |

3.82.14 Detailed Probabilities of TRP82HE3:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 0.89 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| W82HA | 1.00 |
| W82HB2 | 1.00 |
| W82HB3 | 1.00 |
| W82HD1 | 1.00 |
| W82HZ2 | 1.00 |
| W82HZ3 | 1.00 |
| W82HH2 | 1.00 |
| W82HE1 | 1.00 |
| W82HE3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HA | 1.00 | 0.003 | 1.00 | 1.02 |
| TRP82 | HB2 | 1.00 | 0.003 | 1.00 | 0.14 |
| TRP82 | HB3 | 1.00 | 0.002 | 1.00 | 0.15 |
| TRP82 | HD1 | 1.00 | 0.122 | 0.00 | 0.00 |
| TRP82 | HE3 | 1.00 | 0.000 | 1.00 | 1.69 |
| TRP82 | HZ2 | 1.00 | 0.009 | 1.00 | 0.09 |
| TRP82 | HZ3 | 1.00 | 0.007 | 1.00 | 0.99 |
| TRP82 | HH2 | 1.00 | 0.020 | 1.00 | 0.13 |
| TRP82 | HE1 | 1.00 | 0.011 | 1.00 | -95024.00 |

3.82.15 Detailed Probabilities of TRP82HZ2:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| W82HD1 | 1.00 |
| W82HE3 | 1.00 |
| W82HZ3 | 1.00 |
| W82HH2 | 1.00 |
| W82HE1 | 1.00 |
| W82HZ2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HD1 | 1.00 | 0.006 | 1.00 | 0.25 |
| TRP82 | HE3 | 1.00 | 0.081 | 0.00 | 0.00 |
| TRP82 | HZ2 | 1.00 | 0.006 | 1.00 | 6.41 |
| TRP82 | HZ3 | 1.00 | 0.167 | 0.00 | 0.00 |
| TRP82 | HH2 | 1.00 | 0.003 | 1.00 | 0.41 |
| TRP82 | HE1 | 1.00 | 0.008 | 1.00 | -871290.00 |

3.82.16 Detailed Probabilities of TRP82HZ3:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 0.75 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| W82HE3 | 1.00 |
| W82HZ2 | 1.00 |
| W82HH2 | 1.00 |
| W82HZ3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HE3 | 1.00 | 0.000 | 1.00 | 0.27 |
| TRP82 | HZ2 | 1.00 | 0.000 | 1.00 | 0.20 |
| TRP82 | HZ3 | 1.00 | 0.154 | 0.00 | 0.00 |
| TRP82 | HH2 | 1.00 | 0.002 | 1.00 | 1.18 |

3.82.17 Detailed Probabilities of TRP82HH2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| W82HE3 | 1.00 |
| W82HZ2 | 1.00 |
| W82HZ3 | 1.00 |
| W82HE1 | 1.00 |
| W82HH2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HE3 | 1.00 | 0.001 | 1.00 | 0.16 |
| TRP82 | HZ2 | 1.00 | 0.001 | 1.00 | 1.56 |
| TRP82 | HZ3 | 1.00 | 0.005 | 1.00 | 0.20 |
| TRP82 | HH2 | 1.00 | 0.004 | 1.00 | 6.58 |
| TRP82 | HE1 | 1.00 | 0.000 | 1.00 | -146404.00 |

3.82.18 Detailed Probabilities of TRP82H:

Overall probability: 0.970

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP81 | 1.00 | 1.00 |
| TRP82 | 0.94 | 1.00 |
| ASN83 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D81H | 1.00 |
| D81HB2 | 1.00 |
| D81HA | 1.00 |
| D81HB3 | 1.00 |
| W82HA | 1.00 |
| W82HB2 | 1.00 |
| W82HB3 | 1.00 |
| W82HD1 | 0.99 |
| W82H | 1.00 |
| N83H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP81 | HA | 1.00 | 0.005 | 1.00 | 1.03 |
| ASP81 | HB2 | 1.00 | 0.016 | 1.00 | 0.06 |
| ASP81 | HB3 | 1.00 | 0.003 | 1.00 | 0.08 |
| ASP81 | H | 1.00 | 0.006 | 1.00 | -105645.00 |
| TRP82 | HA | 1.00 | 0.033 | 0.70 | 0.00 |
| TRP82 | HB2 | 1.00 | 0.002 | 1.00 | 0.18 |
| TRP82 | HB3 | 1.00 | 0.003 | 1.00 | 0.15 |
| TRP82 | HD1 | 0.99 | 0.003 | 1.00 | 0.25 |
| TRP82 | H | 1.00 | 0.006 | 1.00 | -2069368.00 |
| ASN83 | H | 1.00 | 0.004 | 1.00 | -128089.00 |

3.82.19 Detailed Probabilities of TRP82HE1:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| W82HB2 | 1.00 |
| W82HB3 | 1.00 |
| W82HD1 | 1.00 |
| W82HE3 | 1.00 |
| W82HZ2 | 1.00 |
| W82HH2 | 1.00 |
| W82HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HB2 | 1.00 | 0.439 | 0.00 | 0.00 |
| TRP82 | HB3 | 1.00 | 0.440 | 0.00 | 0.00 |
| TRP82 | HD1 | 1.00 | 0.004 | 1.00 | 0.62 |
| TRP82 | HE3 | 1.00 | 1.147 | 0.00 | 0.00 |
| TRP82 | HZ2 | 1.00 | 0.002 | 1.00 | 0.20 |
| TRP82 | HH2 | 1.00 | 0.334 | 0.00 | 0.00 |
| TRP82 | HE1 | 1.00 | 0.003 | 1.00 | -10815338.00 |
| TRP82 | HA | 0.60 | 0.023 | 1.00 | 0.16 |

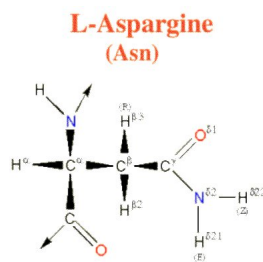
3.83 ASN(83)

Figure 73: Image from the BMRB

Residue probability: 0.854

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|--------------|-------------|---------|--------|---------------------|--------------------|
| C | 176.745 | 175.315 | 1.862 | 0.000 | 0.000 |
| CA 3.83.1 | 56.236 | 53.674 | 5.429 | 0.636 | 1.000 |
| CB 3.83.2 | 37.524 | 38.785 | 5.449 | 1.000 | 1.000 |
| N 3.83.3 | 117.045 | 118.907 | 6.480 | 0.982 | 1.000 |
| ND2 3.83.4 | 114.740 | 112.932 | 14.355 | 1.000 | 1.000 |
| HA 3.83.5 | 4.567 | 4.658 | 0.371 | 0.900 | 1.000 |
| HB2 3.83.6 | 2.956 | 2.800 | 0.341 | 0.875 | 1.000 |
| HB3 3.83.7 | 2.772 | 2.739 | 0.364 | 0.714 | 1.000 |
| H 3.83.8 | 9.661 | 8.328 | 0.633 | 0.636 | 1.000 |
| HD21 3.83.9 | 8.068 | 7.343 | 1.188 | 1.000 | 1.000 |
| HD22 3.83.10 | 7.107 | 7.145 | 1.184 | 0.800 | 1.000 |

3.83.1 Detailed Probabilities of ASN83CA:

Overall probability: 0.636

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 1.00 | 1.00 |
| ASN83 | 0.50 | 1.00 |
| LEU84 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| W82HA | 1.00 |
| N83HB2 | 1.00 |
| N83HB3 | 1.00 |
| N83H | 1.00 |
| N83HD21 | 1.00 |
| N83HD22 | 1.00 |
| N83HA | 1.00 |
| L84HA | 1.00 |
| L84H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HA | 1.00 | 0.025 | 1.00 | 51.32 |
| TRP82 | HB2 | 0.63 | 0.004 | 1.00 | 0.06 |
| TRP82 | HB3 | 0.81 | 0.025 | 1.00 | 0.14 |
| ASN83 | HA | 1.00 | 0.005 | 1.00 | 51.32 |
| ASN83 | HB2 | 1.00 | 0.184 | 0.00 | 0.00 |
| ASN83 | HB3 | 1.00 | 0.000 | 1.00 | 1.22 |
| ASN83 | H | 1.00 | 0.360 | 0.00 | 0.00 |
| ASN83 | HD21 | 1.00 | 0.016 | 1.00 | 0.17 |
| ASN83 | HD22 | 1.00 | 0.238 | 0.00 | 0.00 |
| LEU84 | HA | 1.00 | 0.002 | 1.00 | 0.50 |
| LEU84 | H | 1.00 | 0.077 | 0.00 | 0.00 |

3.83.2 Detailed Probabilities of ASN83CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN83 | 1.00 | 1.00 |
| LEU84 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N83HA | 1.00 |
| N83HB3 | 1.00 |
| N83H | 1.00 |
| N83HD21 | 1.00 |
| N83HD22 | 1.00 |
| N83HB2 | 1.00 |
| L84H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN83 | HA | 1.00 | 0.006 | 1.00 | 0.75 |
| ASN83 | HB2 | 1.00 | 0.002 | 1.00 | 4.46 |
| ASN83 | HB3 | 1.00 | 0.002 | 1.00 | 4.47 |
| ASN83 | H | 1.00 | 0.002 | 1.00 | 0.28 |
| ASN83 | HD21 | 1.00 | 0.001 | 1.00 | 0.28 |
| ASN83 | HD22 | 1.00 | 0.002 | 1.00 | 0.17 |
| LEU84 | H | 1.00 | 0.002 | 1.00 | 0.23 |
| LEU84 | HA | 0.65 | 0.019 | 1.00 | 0.07 |

3.83.3 Detailed Probabilities of ASN83N:

Overall probability: 0.982

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 0.95 | 1.00 |
| ASN83 | 1.00 | 1.00 |
| LEU84 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| W82HB3 | 1.00 |
| W82HA | 1.00 |
| W82HB2 | 1.00 |
| W82H | 1.00 |
| N83HA | 1.00 |
| N83HB2 | 1.00 |
| N83HB3 | 1.00 |
| N83HD21 | 0.98 |
| N83H | 1.00 |
| L84H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HA | 1.00 | 0.032 | 0.80 | 0.00 |
| TRP82 | HB2 | 1.00 | 0.001 | 1.00 | -141336.00 |
| TRP82 | HB3 | 1.00 | 0.005 | 1.00 | -96149.00 |
| TRP82 | H | 1.00 | 0.004 | 1.00 | -128089.00 |
| ASN83 | HA | 1.00 | 0.002 | 1.00 | -624059.00 |
| ASN83 | HB2 | 1.00 | 0.002 | 1.00 | -669271.00 |
| ASN83 | HB3 | 1.00 | 0.001 | 1.00 | -591281.00 |
| ASN83 | H | 1.00 | 0.000 | 1.00 | -1087724.00 |
| ASN83 | HD21 | 0.98 | 0.001 | 1.00 | -99537.00 |
| LEU84 | H | 1.00 | 0.002 | 1.00 | -527826.00 |
| LEU84 | HB2 | 0.65 | 0.020 | 1.00 | -153241.00 |

3.83.4 Detailed Probabilities of ASN83ND2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN83 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N83HA | 1.00 |
| N83HB2 | 1.00 |
| N83HB3 | 1.00 |
| N83H | 0.98 |
| N83HD22 | 1.00 |
| N83HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN83 | HA | 1.00 | 0.005 | 1.00 | -138957.00 |
| ASN83 | HB2 | 1.00 | 0.004 | 1.00 | -686537.00 |
| ASN83 | HB3 | 1.00 | 0.001 | 1.00 | -526449.00 |
| ASN83 | H | 0.98 | 0.008 | 1.00 | -90410.00 |
| ASN83 | HD21 | 1.00 | 0.000 | 1.00 | -4014829.00 |
| ASN83 | HD22 | 1.00 | 0.006 | 1.00 | -3782895.00 |

3.83.5 Detailed Probabilities of ASN83HA:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 0.93 | 1.00 |
| ASN83 | 1.00 | 1.00 |
| LEU84 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| W82HA | 1.00 |
| N83HB2 | 1.00 |
| N83HB3 | 1.00 |
| N83H | 1.00 |
| N83HD21 | 1.00 |
| N83HD22 | 1.00 |
| N83HA | 1.00 |
| L84HA | 1.00 |
| L84H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HA | 1.00 | 0.033 | 0.70 | 0.00 |
| TRP82 | HB2 | 0.63 | 0.024 | 1.00 | 0.32 |
| TRP82 | HB3 | 0.81 | 0.029 | 1.00 | 0.40 |
| TRP82 | H | 0.85 | 0.008 | 1.00 | -1801510.00 |
| ASN83 | HA | 1.00 | 0.005 | 1.00 | 51.32 |
| ASN83 | HB2 | 1.00 | 0.006 | 1.00 | 0.75 |
| ASN83 | HB3 | 1.00 | 0.007 | 1.00 | 1.18 |
| ASN83 | H | 1.00 | 0.002 | 1.00 | -624059.00 |
| ASN83 | HD21 | 1.00 | 0.005 | 1.00 | -138957.00 |
| ASN83 | HD22 | 1.00 | 0.015 | 1.00 | -159602.00 |
| LEU84 | HA | 1.00 | 0.150 | 0.00 | 0.00 |
| LEU84 | H | 1.00 | 0.011 | 1.00 | -813356.00 |
| LEU84 | HB2 | 0.52 | 0.017 | 1.00 | 0.11 |

3.83.6 Detailed Probabilities of ASN83HB2:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN83 | 0.83 | 1.00 |
| LEU84 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N83HA | 1.00 |
| N83HB3 | 1.00 |
| N83H | 1.00 |
| N83HD21 | 1.00 |
| N83HD22 | 1.00 |
| N83HB2 | 1.00 |
| L84H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN83 | HA | 1.00 | 0.184 | 0.00 | 0.00 |
| ASN83 | HB2 | 1.00 | 0.002 | 1.00 | 4.46 |
| ASN83 | HB3 | 1.00 | 0.003 | 1.00 | 4.32 |
| ASN83 | H | 1.00 | 0.002 | 1.00 | -669271.00 |
| ASN83 | HD21 | 1.00 | 0.004 | 1.00 | -686537.00 |
| ASN83 | HD22 | 1.00 | 0.003 | 1.00 | -487345.00 |
| LEU84 | H | 1.00 | 0.004 | 1.00 | -451870.00 |
| LEU84 | HA | 0.65 | 0.000 | 1.00 | 0.08 |

3.83.7 Detailed Probabilities of ASN83HB3:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN83 | 0.83 | 1.00 |
| LEU84 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N83HA | 1.00 |
| N83HB2 | 1.00 |
| N83H | 1.00 |
| N83HD21 | 1.00 |
| N83HD22 | 1.00 |
| N83HB3 | 1.00 |
| L84H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN83 | HA | 1.00 | 0.000 | 1.00 | 1.22 |
| ASN83 | HB2 | 1.00 | 0.002 | 1.00 | 4.47 |
| ASN83 | HB3 | 1.00 | 0.181 | 0.00 | 0.00 |
| ASN83 | H | 1.00 | 0.001 | 1.00 | -591281.00 |
| ASN83 | HD21 | 1.00 | 0.001 | 1.00 | -526449.00 |
| ASN83 | HD22 | 1.00 | 0.000 | 1.00 | -368539.00 |
| LEU84 | H | 1.00 | 0.049 | 0.00 | 0.00 |

3.83.8 Detailed Probabilities of ASN83H:

Overall probability: 0.636

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TRP82 | 0.25 | 1.00 |
| ASN83 | 0.83 | 1.00 |
| LEU84 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| W82HB3 | 1.00 |
| W82HA | 1.00 |
| W82HB2 | 1.00 |
| W82H | 1.00 |
| N83HA | 1.00 |
| N83HB2 | 1.00 |
| N83HB3 | 1.00 |
| N83HD21 | 0.98 |
| N83H | 1.00 |
| L84H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TRP82 | HA | 1.00 | 0.171 | 0.00 | 0.00 |
| TRP82 | HB2 | 1.00 | 0.291 | 0.00 | 0.00 |
| TRP82 | HB3 | 1.00 | 0.292 | 0.00 | 0.00 |
| TRP82 | H | 1.00 | 0.002 | 1.00 | -122598.00 |
| ASN83 | HA | 1.00 | 0.360 | 0.00 | 0.00 |
| ASN83 | HB2 | 1.00 | 0.002 | 1.00 | 0.28 |
| ASN83 | HB3 | 1.00 | 0.000 | 1.00 | 0.25 |
| ASN83 | H | 1.00 | 0.000 | 1.00 | -1087724.00 |
| ASN83 | HD21 | 0.98 | 0.008 | 1.00 | -90410.00 |
| ASN83 | HD22 | 0.63 | 0.007 | 1.00 | -95081.00 |
| LEU84 | H | 1.00 | 0.000 | 1.00 | -464559.00 |

3.83.9 Detailed Probabilities of ASN83HD21:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN83 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N83HA | 1.00 |
| N83HB2 | 1.00 |
| N83HB3 | 1.00 |
| N83H | 0.98 |
| N83HD22 | 1.00 |
| N83HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN83 | HA | 1.00 | 0.016 | 1.00 | 0.17 |
| ASN83 | HB2 | 1.00 | 0.001 | 1.00 | 0.28 |
| ASN83 | HB3 | 1.00 | 0.001 | 1.00 | 0.25 |
| ASN83 | H | 0.98 | 0.001 | 1.00 | -99537.00 |
| ASN83 | HD21 | 1.00 | 0.000 | 1.00 | -4014829.00 |
| ASN83 | HD22 | 1.00 | 0.002 | 1.00 | -3737496.00 |

3.83.10 Detailed Probabilities of ASN83HD22:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN83 | 0.80 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N83HA | 1.00 |
| N83HB2 | 1.00 |
| N83HB3 | 1.00 |
| N83HD21 | 1.00 |
| N83HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN83 | HA | 1.00 | 0.238 | 0.00 | 0.00 |
| ASN83 | HB2 | 1.00 | 0.002 | 1.00 | 0.17 |
| ASN83 | HB3 | 1.00 | 0.004 | 1.00 | 0.15 |
| ASN83 | HD21 | 1.00 | 0.006 | 1.00 | -3782895.00 |
| ASN83 | HD22 | 1.00 | 0.006 | 1.00 | -4779584.00 |

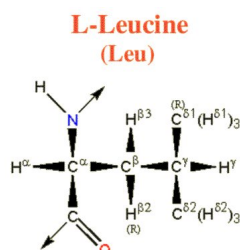
3.84 LEU(84)

Figure 74: Image from the BMRB

Residue probability: 0.891

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 178.149 | 177.056 | 1.929 | 0.000 | 0.000 |
| CA 3.84.1 | 56.004 | 55.735 | 3.802 | 0.818 | 1.000 |
| CB 3.84.2 | 41.447 | 42.389 | 3.750 | 1.000 | 1.000 |
| CG 3.84.3 | 27.385 | 26.892 | 3.086 | 1.000 | 1.000 |
| CD1 3.84.4 | 24.788 | 24.837 | 3.657 | 1.000 | 1.000 |
| CD2 3.84.5 | 22.968 | 24.201 | 3.117 | 0.573 | 1.000 |
| N 3.84.6 | 117.468 | 121.785 | 4.943 | 0.923 | 1.000 |
| HA 3.84.7 | 4.405 | 4.315 | 0.840 | 0.834 | 1.000 |
| HB2 3.84.8 | 1.727 | 1.601 | 0.373 | 0.875 | 1.000 |
| HB3 3.84.9 | 1.947 | 1.508 | 0.398 | 0.778 | 1.000 |
| HG 3.84.10 | 1.705 | 1.510 | 0.340 | 1.000 | 1.000 |
| HD1 3.84.11 | 1.031 | 0.739 | 0.294 | 1.000 | 1.000 |
| HD2 3.84.12 | 0.916 | 0.727 | 0.421 | 0.857 | 1.000 |
| H 3.84.13 | 7.784 | 8.237 | 0.647 | 0.929 | 1.000 |

3.84.1 Detailed Probabilities of LEU84CA:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN83 | 0.50 | 1.00 |
| LEU84 | 1.00 | 1.00 |
| LEU85 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N83HA | 1.00 |
| L84HB2 | 1.00 |
| L84HB3 | 1.00 |
| L84HG | 1.00 |
| L84HD11 | 0.99 |
| L84HD21 | 0.99 |
| L84H | 1.00 |
| L84HA | 1.00 |
| L85H | 1.00 |
| L85HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN83 | HA | 1.00 | 0.150 | 0.00 | 0.00 |
| ASN83 | HB2 | 0.65 | 0.000 | 1.00 | 0.08 |
| LEU84 | HA | 1.00 | 0.012 | 1.00 | 55.95 |
| LEU84 | HB2 | 1.00 | 0.004 | 1.00 | 1.79 |
| LEU84 | HB3 | 1.00 | 0.004 | 1.00 | 1.99 |
| LEU84 | HG | 1.00 | 0.018 | 1.00 | 1.79 |
| LEU84 | HD11 | 0.99 | 0.007 | 1.00 | 0.66 |
| LEU84 | HD21 | 0.99 | 0.001 | 1.00 | 2.46 |
| LEU84 | H | 1.00 | 0.005 | 1.00 | 0.66 |
| LEU85 | HA | 1.00 | 0.187 | 0.00 | 0.00 |
| LEU85 | H | 1.00 | 0.007 | 1.00 | 0.19 |

3.84.2 Detailed Probabilities of LEU84CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU84 | 1.00 | 1.00 |
| LEU85 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L84HA | 1.00 |
| L84HB3 | 1.00 |
| L84HG | 1.00 |
| L84HD11 | 1.00 |
| L84HD21 | 1.00 |
| L84H | 1.00 |
| L84HB2 | 1.00 |
| L85H | 1.00 |

NOESY contacts detailed probability

3.84 LEU(84)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU84 | HA | 1.00 | 0.002 | 1.00 | 1.02 |
| LEU84 | HB2 | 1.00 | 0.007 | 1.00 | 8.50 |
| LEU84 | HB3 | 1.00 | 0.007 | 1.00 | 3.95 |
| LEU84 | HG | 1.00 | 0.015 | 1.00 | 8.50 |
| LEU84 | HD11 | 1.00 | 0.003 | 1.00 | 1.40 |
| LEU84 | HD21 | 1.00 | 0.001 | 1.00 | 1.28 |
| LEU84 | H | 1.00 | 0.000 | 1.00 | 0.73 |
| LEU85 | H | 1.00 | 0.004 | 1.00 | 0.24 |
| LEU85 | HA | 0.65 | 0.020 | 1.00 | 0.11 |

3.84.3 Detailed Probabilities of LEU84CG:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU84 | 1.00 | 1.00 |
| LEU85 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L84HA | 1.00 |
| L84HB2 | 1.00 |
| L84HB3 | 1.00 |
| L84HD11 | 1.00 |
| L84HD21 | 1.00 |
| L84H | 1.00 |
| L84HG | 1.00 |
| L85H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU84 | HA | 1.00 | 0.001 | 1.00 | 0.68 |
| LEU84 | HB2 | 1.00 | 0.017 | 1.00 | 27.01 |
| LEU84 | HB3 | 1.00 | 0.012 | 1.00 | 5.96 |
| LEU84 | HG | 1.00 | 0.005 | 1.00 | 27.01 |
| LEU84 | HD11 | 1.00 | 0.002 | 1.00 | 2.16 |
| LEU84 | HD21 | 1.00 | 0.004 | 1.00 | 3.90 |
| LEU84 | H | 1.00 | 0.000 | 1.00 | 0.91 |
| LEU85 | H | 0.98 | 0.013 | 1.00 | 0.83 |

3.84.4 Detailed Probabilities of LEU84CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU84 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L84HA | 0.99 |
| L84HB2 | 1.00 |
| L84HB3 | 1.00 |
| L84HG | 1.00 |
| L84HD12 | 1.00 |
| L84HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU84 | HA | 0.99 | 0.001 | 1.00 | 0.77 |
| LEU84 | HB2 | 1.00 | 0.013 | 1.00 | 4.61 |
| LEU84 | HB3 | 1.00 | 0.009 | 1.00 | 2.04 |
| LEU84 | HG | 1.00 | 0.009 | 1.00 | 4.61 |
| LEU84 | HD11 | 1.00 | 0.002 | 1.00 | 194.02 |
| LEU84 | HD21 | 1.00 | 0.000 | 1.00 | 8.75 |
| LEU84 | H | 0.86 | 0.003 | 1.00 | 0.58 |

3.84.5 Detailed Probabilities of LEU84CD2:

Overall probability: 0.573

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU84 | 0.57 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L84HA | 0.99 |
| L84HB2 | 1.00 |
| L84HB3 | 1.00 |
| L84HG | 1.00 |
| L84HD11 | 1.00 |
| L84HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU84 | HA | 0.99 | 0.410 | 0.01 | 0.00 |
| LEU84 | HB2 | 1.00 | 0.015 | 1.00 | 4.94 |
| LEU84 | HB3 | 1.00 | 0.235 | 0.00 | 0.00 |
| LEU84 | HG | 1.00 | 0.007 | 1.00 | 4.94 |
| LEU84 | HD11 | 1.00 | 0.001 | 1.00 | 9.13 |
| LEU84 | HD21 | 1.00 | 0.114 | 0.00 | 0.00 |
| LEU84 | H | 0.85 | 0.002 | 1.00 | 0.65 |

3.84.6 Detailed Probabilities of LEU84N:

Overall probability: 0.923

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN83 | 0.75 | 1.00 |
| LEU84 | 1.00 | 1.00 |
| LEU85 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| N83HB2 | 1.00 |
| N83H | 1.00 |
| N83HB3 | 1.00 |
| N83HA | 1.00 |
| L84HA | 1.00 |
| L84HB2 | 1.00 |
| L84HB3 | 1.00 |
| L84HG | 1.00 |
| L84H | 1.00 |
| L85H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN83 | HA | 1.00 | 0.011 | 1.00 | -813356.00 |
| ASN83 | HB2 | 1.00 | 0.004 | 1.00 | -451870.00 |
| ASN83 | HB3 | 1.00 | 0.049 | 0.00 | 0.00 |
| ASN83 | H | 1.00 | 0.000 | 1.00 | -464559.00 |
| LEU84 | HA | 1.00 | 0.001 | 1.00 | -1362954.00 |
| LEU84 | HB2 | 1.00 | 0.015 | 1.00 | -3262282.00 |
| LEU84 | HB3 | 1.00 | 0.011 | 1.00 | -2632994.00 |
| LEU84 | HG | 1.00 | 0.007 | 1.00 | -3262282.00 |
| LEU84 | H | 1.00 | 0.002 | 1.00 | -15949911.00 |
| LEU84 | HD11 | 0.88 | 0.004 | 1.00 | -747725.00 |
| LEU84 | HD21 | 0.87 | 0.002 | 1.00 | -809331.00 |
| LEU85 | H | 1.00 | 0.002 | 1.00 | -3091128.00 |
| LEU85 | HA | 0.93 | 0.026 | 1.00 | -813356.00 |

3.84.7 Detailed Probabilities of LEU84HA:

Overall probability: 0.834

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN83 | 1.00 | 1.00 |
| LEU84 | 0.86 | 1.00 |
| LEU85 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| N83HA | 1.00 |
| L84HB2 | 1.00 |
| L84HB3 | 1.00 |
| L84HG | 1.00 |
| L84HD11 | 0.99 |
| L84HD21 | 0.99 |
| L84H | 1.00 |
| L84HA | 1.00 |
| L85H | 1.00 |
| L85HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN83 | HA | 1.00 | 0.002 | 1.00 | 0.50 |
| ASN83 | HB2 | 0.65 | 0.019 | 1.00 | 0.07 |
| ASN83 | HB3 | 0.87 | 0.006 | 1.00 | 0.12 |
| LEU84 | HA | 1.00 | 0.012 | 1.00 | 55.95 |
| LEU84 | HB2 | 1.00 | 0.002 | 1.00 | 1.02 |
| LEU84 | HB3 | 1.00 | 0.001 | 1.00 | 0.83 |
| LEU84 | HG | 1.00 | 0.001 | 1.00 | 0.68 |
| LEU84 | HD11 | 0.99 | 0.001 | 1.00 | 0.77 |
| LEU84 | HD21 | 0.99 | 0.410 | 0.01 | 0.00 |
| LEU84 | H | 1.00 | 0.001 | 1.00 | -1362954.00 |
| LEU85 | HA | 1.00 | 0.133 | 0.00 | 0.00 |
| LEU85 | H | 1.00 | 0.003 | 1.00 | -663517.00 |

3.84.8 Detailed Probabilities of LEU84HB2:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU84 | 1.00 | 1.00 |
| LEU85 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L84HA | 1.00 |
| L84HB3 | 1.00 |
| L84HG | 1.00 |
| L84HD11 | 1.00 |
| L84HD21 | 1.00 |
| L84H | 1.00 |
| L84HB2 | 1.00 |
| L85H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU84 | HA | 1.00 | 0.004 | 1.00 | 1.79 |
| LEU84 | HB2 | 1.00 | 0.007 | 1.00 | 8.50 |
| LEU84 | HB3 | 1.00 | 0.007 | 1.00 | 5.89 |
| LEU84 | HG | 1.00 | 0.017 | 1.00 | 27.01 |
| LEU84 | HD11 | 1.00 | 0.013 | 1.00 | 4.61 |
| LEU84 | HD21 | 1.00 | 0.015 | 1.00 | 4.94 |
| LEU84 | H | 1.00 | 0.015 | 1.00 | -3262282.00 |
| LEU85 | H | 1.00 | 0.044 | 0.00 | 0.00 |

3.84.9 Detailed Probabilities of LEU84HB3:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU84 | 0.86 | 1.00 |
| LEU85 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L84HA | 1.00 |
| L84HB2 | 1.00 |
| L84HG | 1.00 |
| L84HD11 | 1.00 |
| L84HD21 | 1.00 |
| L84H | 1.00 |
| L84HB3 | 1.00 |
| L85H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU84 | HA | 1.00 | 0.004 | 1.00 | 1.99 |
| LEU84 | HB2 | 1.00 | 0.007 | 1.00 | 3.95 |
| LEU84 | HB3 | 1.00 | 0.008 | 1.00 | 5.91 |
| LEU84 | HG | 1.00 | 0.012 | 1.00 | 5.96 |
| LEU84 | HD11 | 1.00 | 0.009 | 1.00 | 2.04 |
| LEU84 | HD21 | 1.00 | 0.235 | 0.00 | 0.00 |
| LEU84 | H | 1.00 | 0.011 | 1.00 | -2632994.00 |
| LEU85 | H | 1.00 | 0.043 | 0.00 | 0.00 |
| LEU85 | HA | 0.93 | 0.019 | 1.00 | 0.23 |

3.84.10 Detailed Probabilities of LEU84HG:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU84 | 1.00 | 1.00 |
| LEU85 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L84HA | 1.00 |
| L84HB2 | 1.00 |
| L84HB3 | 1.00 |
| L84HD11 | 1.00 |
| L84HD21 | 1.00 |
| L84H | 1.00 |
| L84HG | 1.00 |
| L85H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU84 | HA | 1.00 | 0.018 | 1.00 | 1.79 |
| LEU84 | HB2 | 1.00 | 0.015 | 1.00 | 8.50 |
| LEU84 | HB3 | 1.00 | 0.015 | 1.00 | 5.89 |
| LEU84 | HG | 1.00 | 0.005 | 1.00 | 27.01 |
| LEU84 | HD11 | 1.00 | 0.009 | 1.00 | 4.61 |
| LEU84 | HD21 | 1.00 | 0.007 | 1.00 | 4.94 |
| LEU84 | H | 1.00 | 0.007 | 1.00 | -3262282.00 |
| LEU85 | H | 0.98 | 0.022 | 1.00 | -2851216.00 |

3.84.11 Detailed Probabilities of LEU84HD11:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU84 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L84HA | 0.99 |
| L84HB2 | 1.00 |
| L84HB3 | 1.00 |
| L84HG | 1.00 |
| L84HD12 | 1.00 |
| L84HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU84 | HA | 0.99 | 0.007 | 1.00 | 0.66 |
| LEU84 | HB2 | 1.00 | 0.003 | 1.00 | 1.40 |
| LEU84 | HB3 | 1.00 | 0.003 | 1.00 | 1.35 |
| LEU84 | HG | 1.00 | 0.002 | 1.00 | 2.16 |
| LEU84 | HD11 | 1.00 | 0.002 | 1.00 | 194.02 |
| LEU84 | HD21 | 1.00 | 0.001 | 1.00 | 9.13 |
| LEU84 | H | 0.86 | 0.004 | 1.00 | -747725.00 |

3.84.12 Detailed Probabilities of LEU84HD21:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU84 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L84HA | 0.99 |
| L84HB2 | 1.00 |
| L84HB3 | 1.00 |
| L84HG | 1.00 |
| L84HD11 | 1.00 |
| L84HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU84 | HA | 0.99 | 0.001 | 1.00 | 2.46 |
| LEU84 | HB2 | 1.00 | 0.001 | 1.00 | 1.28 |
| LEU84 | HB3 | 1.00 | 0.001 | 1.00 | 0.94 |
| LEU84 | HG | 1.00 | 0.004 | 1.00 | 3.90 |
| LEU84 | HD11 | 1.00 | 0.000 | 1.00 | 8.75 |
| LEU84 | HD21 | 1.00 | 0.114 | 0.00 | 0.00 |
| LEU84 | H | 0.85 | 0.002 | 1.00 | -809331.00 |

3.84.13 Detailed Probabilities of LEU84H:

Overall probability: 0.929

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASN83 | 0.75 | 1.00 |
| LEU84 | 1.00 | 1.00 |
| LEU85 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| N83HB2 | 1.00 |
| N83H | 1.00 |
| N83HB3 | 1.00 |
| N83HA | 1.00 |
| L84HA | 1.00 |
| L84HB2 | 1.00 |
| L84HB3 | 1.00 |
| L84HG | 1.00 |
| L84H | 1.00 |
| L85H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASN83 | HA | 1.00 | 0.077 | 0.00 | 0.00 |
| ASN83 | HB2 | 1.00 | 0.002 | 1.00 | 0.23 |
| ASN83 | HB3 | 1.00 | 0.000 | 1.00 | 0.20 |
| ASN83 | H | 1.00 | 0.002 | 1.00 | -527826.00 |
| LEU84 | HA | 1.00 | 0.005 | 1.00 | 0.66 |
| LEU84 | HB2 | 1.00 | 0.000 | 1.00 | 0.73 |
| LEU84 | HB3 | 1.00 | 0.001 | 1.00 | 1.06 |
| LEU84 | HG | 1.00 | 0.000 | 1.00 | 0.91 |
| LEU84 | H | 1.00 | 0.002 | 1.00 | -15949911.00 |
| LEU84 | HD11 | 0.88 | 0.003 | 1.00 | 0.58 |
| LEU84 | HD21 | 0.87 | 0.002 | 1.00 | 0.65 |
| LEU85 | H | 1.00 | 0.002 | 1.00 | -3151074.00 |
| LEU85 | HA | 0.93 | 0.027 | 1.00 | 0.34 |
| LEU85 | HB2 | 0.64 | 0.010 | 1.00 | 0.06 |

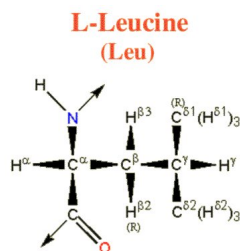
3.85 LEU(85)

Figure 75: Image from the BMRB

Residue probability: 0.853

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 177.473 | 177.056 | 1.929 | 0.000 | 0.000 |
| CA 3.85.1 | 56.544 | 55.735 | 3.802 | 0.567 | 1.000 |
| CB 3.85.2 | 45.136 | 42.389 | 3.750 | 1.000 | 1.000 |
| CG 3.85.3 | 28.122 | 26.892 | 3.086 | 0.625 | 1.000 |
| CD1 3.85.4 | 25.912 | 24.837 | 3.657 | 1.000 | 1.000 |
| CD2 3.85.5 | 24.399 | 24.201 | 3.117 | 1.000 | 1.000 |
| N 3.85.6 | 119.164 | 121.785 | 4.943 | 0.875 | 1.000 |
| HA 3.85.7 | 4.604 | 4.315 | 0.840 | 0.908 | 1.000 |
| HB2 3.85.8 | 1.666 | 1.601 | 0.373 | 0.850 | 1.000 |
| HB3 3.85.9 | 1.894 | 1.508 | 0.398 | 0.875 | 1.000 |
| HG 3.85.10 | 1.678 | 1.510 | 0.340 | 0.875 | 1.000 |
| HD1 3.85.11 | 0.611 | 0.739 | 0.294 | 0.715 | 1.000 |
| HD2 3.85.12 | 0.789 | 0.727 | 0.421 | 0.857 | 1.000 |
| H 3.85.13 | 7.417 | 8.237 | 0.647 | 0.941 | 1.000 |

3.85.1 Detailed Probabilities of LEU85CA:

Overall probability: 0.567

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU84 | 0.67 | 1.00 |
| LEU85 | 0.69 | 1.00 |
| LYS86 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L84HA | 1.00 |
| L85HB2 | 1.00 |
| L85HB3 | 1.00 |
| L85HG | 1.00 |
| L85HD11 | 0.99 |
| L85HD21 | 0.99 |
| L85H | 1.00 |
| L85HA | 1.00 |
| K86HA | 1.00 |
| K86H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU84 | HA | 1.00 | 0.133 | 0.00 | 0.00 |
| LEU84 | HB3 | 0.93 | 0.019 | 1.00 | 0.23 |
| LEU84 | H | 0.93 | 0.027 | 1.00 | 0.34 |
| LEU85 | HA | 1.00 | 0.032 | 0.80 | 0.00 |
| LEU85 | HB2 | 1.00 | 0.012 | 1.00 | 1.69 |
| LEU85 | HB3 | 1.00 | 0.008 | 1.00 | 0.36 |
| LEU85 | HG | 1.00 | 0.000 | 1.00 | 1.69 |
| LEU85 | HD11 | 0.99 | 0.049 | 0.01 | 0.00 |
| LEU85 | HD21 | 0.99 | 0.000 | 1.00 | 1.65 |
| LEU85 | H | 1.00 | 0.198 | 0.00 | 0.00 |
| LYS86 | HA | 1.00 | 0.203 | 0.00 | 0.00 |
| LYS86 | H | 1.00 | 0.225 | 0.00 | 0.00 |

3.85.2 Detailed Probabilities of LEU85CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU85 | 1.00 | 1.00 |
| LYS86 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L85HA | 1.00 |
| L85HB3 | 1.00 |
| L85HG | 1.00 |
| L85HD11 | 1.00 |
| L85HD21 | 1.00 |
| L85H | 1.00 |
| L85HB2 | 1.00 |
| K86H | 1.00 |

NOESY contacts detailed probability

3.85 LEU(85)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU85 | HA | 1.00 | 0.004 | 1.00 | 0.66 |
| LEU85 | HB2 | 1.00 | 0.009 | 1.00 | 3.20 |
| LEU85 | HB3 | 1.00 | 0.007 | 1.00 | 1.42 |
| LEU85 | HG | 1.00 | 0.003 | 1.00 | 3.20 |
| LEU85 | HD11 | 1.00 | 0.003 | 1.00 | 0.51 |
| LEU85 | HD21 | 1.00 | 0.005 | 1.00 | 0.50 |
| LEU85 | H | 1.00 | 0.003 | 1.00 | 0.33 |
| LYS86 | H | 1.00 | 0.003 | 1.00 | 0.17 |

3.85.3 Detailed Probabilities of LEU85CG:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU85 | 0.57 | 1.00 |
| LYS86 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L85HA | 1.00 |
| L85HB2 | 1.00 |
| L85HB3 | 1.00 |
| L85HD11 | 1.00 |
| L85HD21 | 1.00 |
| L85H | 1.00 |
| L85HG | 1.00 |
| K86H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU85 | HA | 1.00 | 0.006 | 1.00 | 1.02 |
| LEU85 | HB2 | 1.00 | 0.087 | 0.00 | 0.00 |
| LEU85 | HB3 | 1.00 | 0.007 | 1.00 | 1.49 |
| LEU85 | HG | 1.00 | 0.099 | 0.00 | 0.00 |
| LEU85 | HD11 | 1.00 | 0.174 | 0.00 | 0.00 |
| LEU85 | HD21 | 1.00 | 0.004 | 1.00 | 1.49 |
| LEU85 | H | 1.00 | 0.000 | 1.00 | 0.77 |
| LYS86 | H | 0.98 | 0.003 | 1.00 | 0.22 |

3.85.4 Detailed Probabilities of LEU85CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU85 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L85HA | 0.99 |
| L85HB2 | 1.00 |
| L85HB3 | 1.00 |
| L85HG | 1.00 |
| L85HD12 | 1.00 |
| L85HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU85 | HA | 0.99 | 0.004 | 1.00 | 1.04 |
| LEU85 | HB2 | 1.00 | 0.011 | 1.00 | 2.86 |
| LEU85 | HB3 | 1.00 | 0.002 | 1.00 | 1.33 |
| LEU85 | HG | 1.00 | 0.001 | 1.00 | 2.86 |
| LEU85 | HD11 | 1.00 | 0.002 | 1.00 | 110.72 |
| LEU85 | HD21 | 1.00 | 0.008 | 1.00 | 4.33 |
| LEU85 | H | 0.86 | 0.002 | 1.00 | 0.60 |

3.85.5 Detailed Probabilities of LEU85CD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU85 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L85HA | 0.99 |
| L85HB2 | 1.00 |
| L85HB3 | 1.00 |
| L85HG | 1.00 |
| L85HD11 | 1.00 |
| L85HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU85 | HA | 0.99 | 0.004 | 1.00 | 2.57 |
| LEU85 | HB2 | 1.00 | 0.011 | 1.00 | 3.03 |
| LEU85 | HB3 | 1.00 | 0.004 | 1.00 | 1.02 |
| LEU85 | HG | 1.00 | 0.001 | 1.00 | 3.03 |
| LEU85 | HD11 | 1.00 | 0.003 | 1.00 | 4.37 |
| LEU85 | HD21 | 1.00 | 0.003 | 1.00 | 151.94 |
| LEU85 | H | 0.85 | 0.005 | 1.00 | 0.63 |

3.85.6 Detailed Probabilities of LEU85N:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU84 | 0.71 | 1.00 |
| LEU85 | 1.00 | 1.00 |
| LYS86 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L84HB3 | 1.00 |
| L84HB2 | 1.00 |
| L84HA | 1.00 |
| L84H | 1.00 |
| L84HG | 0.98 |
| L85HA | 1.00 |
| L85HB2 | 1.00 |
| L85HB3 | 1.00 |
| L85HG | 1.00 |
| L85H | 1.00 |
| K86H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU84 | HA | 1.00 | 0.003 | 1.00 | -663517.00 |
| LEU84 | HB2 | 1.00 | 0.044 | 0.00 | 0.00 |
| LEU84 | HB3 | 1.00 | 0.043 | 0.00 | 0.00 |
| LEU84 | HG | 0.98 | 0.022 | 1.00 | -2851216.00 |
| LEU84 | H | 1.00 | 0.002 | 1.00 | -3151074.00 |
| LEU84 | HD11 | 0.53 | 0.009 | 1.00 | -208930.00 |
| LEU84 | HD21 | 0.58 | 0.028 | 1.00 | -471607.00 |
| LEU85 | HA | 1.00 | 0.008 | 1.00 | -1920018.00 |
| LEU85 | HB2 | 1.00 | 0.017 | 1.00 | -2851216.00 |
| LEU85 | HB3 | 1.00 | 0.010 | 1.00 | -2040722.00 |
| LEU85 | HG | 1.00 | 0.005 | 1.00 | -2851216.00 |
| LEU85 | H | 1.00 | 0.001 | 1.00 | -13629436.00 |
| LEU85 | HD11 | 0.88 | 0.005 | 1.00 | -805266.00 |
| LEU85 | HD21 | 0.87 | 0.000 | 1.00 | -562560.00 |
| LYS86 | H | 1.00 | 0.001 | 1.00 | -2656679.00 |
| LYS86 | HA | 0.89 | 0.004 | 1.00 | -152125.00 |

3.85.7 Detailed Probabilities of LEU85HA:

Overall probability: 0.908

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU84 | 0.75 | 1.00 |
| LEU85 | 0.97 | 1.00 |
| LYS86 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L84HA | 1.00 |
| L85HB2 | 1.00 |
| L85HB3 | 1.00 |
| L85HG | 1.00 |
| L85HD11 | 0.99 |
| L85HD21 | 0.99 |
| L85H | 1.00 |
| L85HA | 1.00 |
| K86HA | 1.00 |
| K86H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU84 | HA | 1.00 | 0.187 | 0.00 | 0.00 |
| LEU84 | HB2 | 0.65 | 0.020 | 1.00 | 0.11 |
| LEU84 | HB3 | 0.93 | 0.023 | 1.00 | 0.09 |
| LEU84 | H | 0.93 | 0.026 | 1.00 | -813356.00 |
| LEU85 | HA | 1.00 | 0.032 | 0.80 | 0.00 |
| LEU85 | HB2 | 1.00 | 0.004 | 1.00 | 0.66 |
| LEU85 | HB3 | 1.00 | 0.004 | 1.00 | 0.54 |
| LEU85 | HG | 1.00 | 0.006 | 1.00 | 1.02 |
| LEU85 | HD11 | 0.99 | 0.004 | 1.00 | 1.04 |
| LEU85 | HD21 | 0.99 | 0.004 | 1.00 | 2.57 |
| LEU85 | H | 1.00 | 0.008 | 1.00 | -1920018.00 |
| LYS86 | HA | 1.00 | 0.006 | 1.00 | 0.07 |
| LYS86 | H | 1.00 | 0.017 | 1.00 | -874399.00 |

3.85.8 Detailed Probabilities of LEU85HB2:

Overall probability: 0.850

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU85 | 0.86 | 1.00 |
| LYS86 | 0.80 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L85HA | 1.00 |
| L85HB3 | 1.00 |
| L85HG | 1.00 |
| L85HD11 | 1.00 |
| L85HD21 | 1.00 |
| L85H | 1.00 |
| L85HB2 | 1.00 |
| K86H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU85 | HA | 1.00 | 0.012 | 1.00 | 1.69 |
| LEU85 | HB2 | 1.00 | 0.009 | 1.00 | 3.20 |
| LEU85 | HB3 | 1.00 | 0.007 | 1.00 | 2.01 |
| LEU85 | HG | 1.00 | 0.087 | 0.00 | 0.00 |
| LEU85 | HD11 | 1.00 | 0.011 | 1.00 | 2.86 |
| LEU85 | HD21 | 1.00 | 0.011 | 1.00 | 3.03 |
| LEU85 | H | 1.00 | 0.017 | 1.00 | -2851216.00 |
| LYS86 | H | 1.00 | 0.032 | 0.80 | 0.00 |

3.85.9 Detailed Probabilities of LEU85HB3:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU85 | 1.00 | 1.00 |
| LYS86 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L85HA | 1.00 |
| L85HB2 | 1.00 |
| L85HG | 1.00 |
| L85HD11 | 1.00 |
| L85HD21 | 1.00 |
| L85H | 1.00 |
| L85HB3 | 1.00 |
| K86H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU85 | HA | 1.00 | 0.008 | 1.00 | 0.36 |
| LEU85 | HB2 | 1.00 | 0.007 | 1.00 | 1.42 |
| LEU85 | HB3 | 1.00 | 0.003 | 1.00 | 1.60 |
| LEU85 | HG | 1.00 | 0.007 | 1.00 | 1.49 |
| LEU85 | HD11 | 1.00 | 0.002 | 1.00 | 1.33 |
| LEU85 | HD21 | 1.00 | 0.004 | 1.00 | 1.02 |
| LEU85 | H | 1.00 | 0.010 | 1.00 | -2040722.00 |
| LYS86 | H | 1.00 | 0.067 | 0.00 | 0.00 |

3.85.10 Detailed Probabilities of LEU85HG:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU85 | 0.86 | 1.00 |
| LYS86 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L85HA | 1.00 |
| L85HB2 | 1.00 |
| L85HB3 | 1.00 |
| L85HD11 | 1.00 |
| L85HD21 | 1.00 |
| L85H | 1.00 |
| L85HG | 1.00 |
| K86H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU85 | HA | 1.00 | 0.000 | 1.00 | 1.69 |
| LEU85 | HB2 | 1.00 | 0.003 | 1.00 | 3.20 |
| LEU85 | HB3 | 1.00 | 0.005 | 1.00 | 2.01 |
| LEU85 | HG | 1.00 | 0.099 | 0.00 | 0.00 |
| LEU85 | HD11 | 1.00 | 0.001 | 1.00 | 2.86 |
| LEU85 | HD21 | 1.00 | 0.001 | 1.00 | 3.03 |
| LEU85 | H | 1.00 | 0.005 | 1.00 | -2851216.00 |
| LYS86 | H | 0.98 | 0.020 | 1.00 | -988804.00 |

3.85.11 Detailed Probabilities of LEU85HD11:

Overall probability: 0.715

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU85 | 0.72 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L85HA | 0.99 |
| L85HB2 | 1.00 |
| L85HB3 | 1.00 |
| L85HG | 1.00 |
| L85HD12 | 1.00 |
| L85HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU85 | HA | 0.99 | 0.049 | 0.01 | 0.00 |
| LEU85 | HB2 | 1.00 | 0.003 | 1.00 | 0.51 |
| LEU85 | HB3 | 1.00 | 0.003 | 1.00 | 0.47 |
| LEU85 | HG | 1.00 | 0.174 | 0.00 | 0.00 |
| LEU85 | HD11 | 1.00 | 0.002 | 1.00 | 110.72 |
| LEU85 | HD21 | 1.00 | 0.003 | 1.00 | 4.37 |
| LEU85 | H | 0.86 | 0.005 | 1.00 | -805266.00 |

3.85.12 Detailed Probabilities of LEU85HD21:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU85 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L85HA | 0.99 |
| L85HB2 | 1.00 |
| L85HB3 | 1.00 |
| L85HG | 1.00 |
| L85HD11 | 1.00 |
| L85HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU85 | HA | 0.99 | 0.000 | 1.00 | 1.65 |
| LEU85 | HB2 | 1.00 | 0.005 | 1.00 | 0.50 |
| LEU85 | HB3 | 1.00 | 0.066 | 0.00 | 0.00 |
| LEU85 | HG | 1.00 | 0.004 | 1.00 | 1.49 |
| LEU85 | HD11 | 1.00 | 0.008 | 1.00 | 4.33 |
| LEU85 | HD21 | 1.00 | 0.003 | 1.00 | 151.94 |
| LEU85 | H | 0.85 | 0.000 | 1.00 | -562560.00 |

3.85.13 Detailed Probabilities of LEU85H:

Overall probability: 0.941

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU84 | 1.00 | 1.00 |
| LEU85 | 0.86 | 1.00 |
| LYS86 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L84HB3 | 1.00 |
| L84HB2 | 1.00 |
| L84HA | 1.00 |
| L84H | 1.00 |
| L84HG | 0.98 |
| L85HA | 1.00 |
| L85HB2 | 1.00 |
| L85HB3 | 1.00 |
| L85HG | 1.00 |
| L85H | 1.00 |
| K86H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU84 | HA | 1.00 | 0.007 | 1.00 | 0.19 |
| LEU84 | HB2 | 1.00 | 0.004 | 1.00 | 0.24 |
| LEU84 | HB3 | 1.00 | 0.005 | 1.00 | 0.34 |
| LEU84 | HG | 0.98 | 0.013 | 1.00 | 0.83 |
| LEU84 | H | 1.00 | 0.002 | 1.00 | -3091128.00 |
| LEU84 | HD11 | 0.53 | 0.005 | 1.00 | 0.19 |
| LEU84 | HD21 | 0.58 | 0.009 | 1.00 | 0.24 |
| LEU85 | HA | 1.00 | 0.198 | 0.00 | 0.00 |
| LEU85 | HB2 | 1.00 | 0.003 | 1.00 | 0.33 |
| LEU85 | HB3 | 1.00 | 0.002 | 1.00 | 0.42 |
| LEU85 | HG | 1.00 | 0.000 | 1.00 | 0.77 |
| LEU85 | H | 1.00 | 0.001 | 1.00 | -13629436.00 |
| LEU85 | HD11 | 0.88 | 0.002 | 1.00 | 0.60 |
| LEU85 | HD21 | 0.87 | 0.005 | 1.00 | 0.63 |
| LYS86 | H | 1.00 | 0.001 | 1.00 | -2185830.00 |
| LYS86 | HA | 0.89 | 0.020 | 1.00 | 0.10 |
| LYS86 | HB2 | 0.58 | 0.002 | 1.00 | 0.06 |

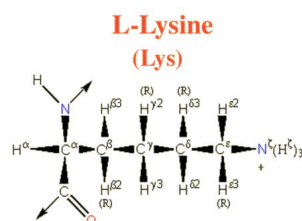


Figure 76: Image from the BMRB

Residue probability: 0.763
Residue probability confidence: 0.943

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | NA | – | – | 0.000 | 0.000 |
| CA 3.86.1 | 62.647 | 57.014 | 3.028 | 0.690 | 1.000 |
| CB 3.86.2 | 30.740 | 32.981 | 3.186 | 0.769 | 1.000 |
| CG 3.86.3 | 27.210 | 24.941 | 1.956 | 0.770 | 0.909 |
| CD 3.86.4 | 29.454 | 29.020 | 2.193 | 0.889 | 0.900 |
| CE 3.86.5 | 41.525 | 41.893 | 1.492 | 0.764 | 0.889 |
| N 3.86.6 | 116.742 | 120.954 | 4.210 | 0.863 | 1.000 |
| NZ | NA | – | – | 0.000 | 0.000 |
| HA 3.86.7 | 3.804 | 4.262 | 0.489 | 0.500 | 1.000 |
| HB2 3.86.8 | 1.756 | 1.774 | 0.365 | 0.394 | 1.000 |
| HB3 3.86.9 | 1.962 | 1.742 | 0.385 | 0.962 | 1.000 |
| HG2 3.86.10 | 1.252 | 1.358 | 0.344 | 0.900 | 0.909 |
| HG3 3.86.11 | 1.962 | 1.343 | 0.357 | 0.950 | 0.909 |
| HD2 3.86.12 | 1.706 | 1.614 | 0.957 | 0.602 | 0.900 |
| HD3 3.86.13 | 1.704 | 1.595 | 0.387 | 0.602 | 0.900 |
| HE2 3.86.14 | 2.802 | 2.907 | 0.230 | 0.791 | 0.889 |
| HE3 3.86.15 | 2.768 | 2.901 | 0.241 | 0.890 | 0.889 |
| H 3.86.16 | 8.659 | 8.185 | 0.605 | 0.867 | 1.000 |
| HZ | NA | – | – | 0.000 | 0.000 |

3.86.1 Detailed Probabilities of LYS86CA:

Overall probability: 0.690
Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU85 | 1.00 | 1.00 |
| LYS86 | 0.70 | 1.00 |
| PRO87 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L85HA | 1.00 |
| K86HB2 | 1.00 |
| K86HB3 | 1.00 |
| K86HG2 | 1.00 |
| K86HG3 | 1.00 |
| K86HD2 | 0.98 |
| K86HD3 | 0.98 |
| K86H | 1.00 |
| K86HA | 1.00 |
| P87HD3 | 1.00 |
| P87HA | 1.00 |
| P87HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU85 | HA | 1.00 | 0.006 | 1.00 | 0.07 |
| LEU85 | H | 0.89 | 0.020 | 1.00 | 0.10 |
| LYS86 | HA | 1.00 | 0.102 | 0.00 | 0.00 |
| LYS86 | HB2 | 1.00 | 0.007 | 1.00 | 0.52 |
| LYS86 | HB3 | 1.00 | 0.001 | 1.00 | 0.76 |
| LYS86 | HG2 | 1.00 | 0.005 | 1.00 | 0.46 |
| LYS86 | HG3 | 1.00 | 0.001 | 1.00 | 0.76 |
| LYS86 | HD2 | 0.98 | 0.043 | 0.02 | 0.00 |
| LYS86 | HD3 | 0.98 | 0.045 | 0.02 | 0.00 |
| LYS86 | H | 1.00 | 0.005 | 1.00 | 0.40 |
| LYS86 | HE2 | 0.77 | 0.019 | 1.00 | 0.05 |
| LYS86 | HE3 | 0.76 | 0.015 | 1.00 | 0.05 |
| PRO87 | HA | 1.00 | 0.311 | 0.00 | 0.00 |
| PRO87 | HD2 | 1.00 | 0.045 | 0.00 | 0.00 |
| PRO87 | HD3 | 1.00 | 0.000 | 1.00 | 0.05 |
| PRO87 | HG2 | 0.93 | 0.009 | 1.00 | 0.76 |

3.86.2 Detailed Probabilities of LYS86CB:

Overall probability: 0.769

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS86 | 0.70 | 1.00 |
| PRO87 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K86HA | 1.00 |
| K86HB2 | 1.00 |
| K86HG2 | 1.00 |
| K86HG3 | 1.00 |
| K86HD2 | 1.00 |
| K86HD3 | 1.00 |
| K86HE2 | 0.99 |
| K86HE3 | 0.99 |
| K86H | 1.00 |
| K86HB3 | 1.00 |
| P87HD2 | 0.99 |
| P87HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS86 | HA | 1.00 | 0.150 | 0.00 | 0.00 |
| LYS86 | HB2 | 1.00 | 0.006 | 1.00 | 1.28 |
| LYS86 | HB3 | 1.00 | 0.012 | 1.00 | 29.96 |
| LYS86 | HG2 | 1.00 | 0.015 | 1.00 | 0.86 |
| LYS86 | HG3 | 1.00 | 0.012 | 1.00 | 29.96 |
| LYS86 | HD2 | 1.00 | 0.044 | 0.00 | 0.00 |
| LYS86 | HD3 | 1.00 | 0.046 | 0.00 | 0.00 |
| LYS86 | HE2 | 0.99 | 0.022 | 1.00 | 0.11 |
| LYS86 | HE3 | 0.99 | 0.012 | 1.00 | 0.11 |
| LYS86 | H | 1.00 | 0.007 | 1.00 | 0.33 |
| PRO87 | HD2 | 0.99 | 0.003 | 1.00 | 0.35 |
| PRO87 | HD3 | 1.00 | 0.002 | 1.00 | 0.22 |
| PRO87 | HG2 | 0.53 | 0.020 | 1.00 | 29.96 |

3.86.3 Detailed Probabilities of LYS86CG:

Overall probability: 0.770

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS86 | 0.77 | 0.91 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K86HA | 1.00 |
| K86HB2 | 1.00 |
| K86HB3 | 1.00 |
| K86HG3 | 1.00 |
| K86HD2 | 1.00 |
| K86HD3 | 1.00 |
| K86HE2 | 1.00 |
| K86HE3 | 1.00 |
| K86H | 1.00 |
| K86HZ2 | 1.00 |
| K86HG2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS86 | HA | 1.00 | 0.010 | 1.00 | 0.26 |
| LYS86 | HB2 | 1.00 | 0.033 | 0.70 | 0.00 |
| LYS86 | HB3 | 1.00 | 0.007 | 1.00 | 1.71 |
| LYS86 | HG2 | 1.00 | 0.018 | 1.00 | 10.96 |
| LYS86 | HG3 | 1.00 | 0.007 | 1.00 | 1.71 |
| LYS86 | HD2 | 1.00 | 0.083 | 0.00 | 0.00 |
| LYS86 | HD3 | 1.00 | 0.085 | 0.00 | 0.00 |
| LYS86 | HE2 | 1.00 | 0.025 | 1.00 | 0.15 |
| LYS86 | HE3 | 1.00 | 0.009 | 1.00 | 0.15 |
| LYS86 | H | 1.00 | 0.001 | 1.00 | 0.14 |

3.86.4 Detailed Probabilities of LYS86CD:

Overall probability: 0.889

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS86 | 0.89 | 0.90 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K86HA | 0.98 |
| K86HB2 | 1.00 |
| K86HB3 | 1.00 |
| K86HG2 | 1.00 |
| K86HG3 | 1.00 |
| K86HD2 | 1.00 |
| K86HE2 | 1.00 |
| K86HE3 | 1.00 |
| K86HZ2 | 1.00 |
| K86HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS86 | HA | 0.98 | 0.023 | 1.00 | 0.80 |
| LYS86 | HB2 | 1.00 | 0.049 | 0.00 | 0.00 |
| LYS86 | HB3 | 1.00 | 0.002 | 1.00 | 1.24 |
| LYS86 | HG2 | 1.00 | 0.002 | 1.00 | 0.66 |
| LYS86 | HG3 | 1.00 | 0.002 | 1.00 | 1.24 |
| LYS86 | HD2 | 1.00 | 0.001 | 1.00 | 20.46 |
| LYS86 | HD3 | 1.00 | 0.003 | 1.00 | 20.46 |
| LYS86 | HE2 | 1.00 | 0.023 | 1.00 | 0.79 |
| LYS86 | HE3 | 1.00 | 0.011 | 1.00 | 0.79 |

3.86.5 Detailed Probabilities of LYS86CE:

Overall probability: 0.764

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS86 | 0.76 | 0.89 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K86HB2 | 0.99 |
| K86HB3 | 0.99 |
| K86HG2 | 1.00 |
| K86HG3 | 1.00 |
| K86HD2 | 1.00 |
| K86HD3 | 1.00 |
| K86HE2 | 1.00 |
| K86HZ2 | 1.00 |
| K86HE3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS86 | HB2 | 0.99 | 0.053 | 0.01 | 0.00 |
| LYS86 | HB3 | 0.99 | 0.001 | 1.00 | 0.45 |
| LYS86 | HG2 | 1.00 | 0.016 | 1.00 | 0.58 |
| LYS86 | HG3 | 1.00 | 0.001 | 1.00 | 0.45 |
| LYS86 | HD2 | 1.00 | 0.003 | 1.00 | 0.87 |
| LYS86 | HD3 | 1.00 | 0.001 | 1.00 | 0.87 |
| LYS86 | HE2 | 1.00 | 0.039 | 0.10 | 0.00 |
| LYS86 | HE3 | 1.00 | 0.005 | 1.00 | 25.44 |

3.86.6 Detailed Probabilities of LYS86N:

Overall probability: 0.863

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU85 | 0.80 | 1.00 |
| LYS86 | 0.88 | 1.00 |
| PRO87 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L85HA | 1.00 |
| L85H | 1.00 |
| L85HB3 | 1.00 |
| L85HB2 | 1.00 |
| L85HG | 0.98 |
| K86HA | 1.00 |
| K86HB2 | 1.00 |
| K86HB3 | 1.00 |
| K86HG2 | 1.00 |
| K86HG3 | 1.00 |
| K86H | 1.00 |
| P87HD2 | 0.99 |
| P87HD3 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU85 | HA | 1.00 | 0.017 | 1.00 | -874399.00 |
| LEU85 | HB2 | 1.00 | 0.032 | 0.80 | 0.00 |
| LEU85 | HB3 | 1.00 | 0.067 | 0.00 | 0.00 |
| LEU85 | HG | 0.98 | 0.020 | 1.00 | -988804.00 |
| LEU85 | H | 1.00 | 0.001 | 1.00 | -2185830.00 |
| LEU85 | HD11 | 0.52 | 0.005 | 1.00 | -215311.00 |
| LYS86 | HA | 1.00 | 0.000 | 1.00 | -801265.00 |
| LYS86 | HB2 | 1.00 | 0.058 | 0.00 | 0.00 |
| LYS86 | HB3 | 1.00 | 0.001 | 1.00 | -2185740.00 |
| LYS86 | HG2 | 1.00 | 0.002 | 1.00 | -370801.00 |
| LYS86 | HG3 | 1.00 | 0.001 | 1.00 | -2185740.00 |
| LYS86 | H | 1.00 | 0.001 | 1.00 | -8587671.00 |
| LYS86 | HD2 | 0.88 | 0.008 | 1.00 | -988804.00 |
| LYS86 | HD3 | 0.87 | 0.006 | 1.00 | -988804.00 |
| PRO87 | HD2 | 0.99 | 0.005 | 1.00 | -717663.00 |
| PRO87 | HD3 | 0.99 | 0.004 | 1.00 | -587899.00 |

3.86.7 Detailed Probabilities of LYS86HA:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU85 | 0.67 | 1.00 |
| LYS86 | 0.50 | 1.00 |
| PRO87 | 0.33 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L85HA | 1.00 |
| K86HB2 | 1.00 |
| K86HB3 | 1.00 |
| K86HG2 | 1.00 |
| K86HG3 | 1.00 |
| K86HD2 | 0.98 |
| K86HD3 | 0.98 |
| K86H | 1.00 |
| K86HA | 1.00 |
| P87HD3 | 1.00 |
| P87HA | 1.00 |
| P87HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU85 | HA | 1.00 | 0.203 | 0.00 | 0.00 |
| LEU85 | HB3 | 0.90 | 0.011 | 1.00 | 0.06 |
| LEU85 | H | 0.89 | 0.004 | 1.00 | -152125.00 |
| LYS86 | HA | 1.00 | 0.102 | 0.00 | 0.00 |
| LYS86 | HB2 | 1.00 | 0.147 | 0.00 | 0.00 |
| LYS86 | HB3 | 1.00 | 0.150 | 0.00 | 0.00 |
| LYS86 | HG2 | 1.00 | 0.010 | 1.00 | 0.26 |
| LYS86 | HG3 | 1.00 | 0.697 | 0.00 | 0.00 |
| LYS86 | HD2 | 0.98 | 0.023 | 1.00 | 0.80 |
| LYS86 | HD3 | 0.98 | 0.023 | 1.00 | 0.80 |
| LYS86 | H | 1.00 | 0.000 | 1.00 | -801265.00 |
| PRO87 | HA | 1.00 | 0.130 | 0.00 | 0.00 |
| PRO87 | HD2 | 1.00 | 0.147 | 0.00 | 0.00 |
| PRO87 | HD3 | 1.00 | 0.026 | 1.00 | 0.27 |

3.86.8 Detailed Probabilities of LYS86HB2:

Overall probability: 0.394

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS86 | 0.27 | 1.00 |
| PRO87 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K86HA | 1.00 |
| K86HB3 | 1.00 |
| K86HG2 | 1.00 |
| K86HG3 | 1.00 |
| K86HD2 | 1.00 |
| K86HD3 | 1.00 |
| K86HE2 | 0.98 |
| K86HE3 | 0.99 |
| K86H | 1.00 |
| K86HB2 | 1.00 |
| P87HD2 | 0.99 |
| P87HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS86 | HA | 1.00 | 0.007 | 1.00 | 0.52 |
| LYS86 | HB2 | 1.00 | 0.209 | 0.00 | 0.00 |
| LYS86 | HB3 | 1.00 | 0.006 | 1.00 | 1.28 |
| LYS86 | HG2 | 1.00 | 0.033 | 0.70 | 0.00 |
| LYS86 | HG3 | 1.00 | 0.399 | 0.00 | 0.00 |
| LYS86 | HD2 | 1.00 | 0.049 | 0.00 | 0.00 |
| LYS86 | HD3 | 1.00 | 0.049 | 0.00 | 0.00 |
| LYS86 | HE2 | 0.98 | 0.053 | 0.02 | 0.00 |
| LYS86 | HE3 | 0.99 | 0.053 | 0.01 | 0.00 |
| LYS86 | H | 1.00 | 0.058 | 0.00 | 0.00 |
| PRO87 | HD2 | 0.99 | 0.016 | 1.00 | 1.06 |
| PRO87 | HD3 | 1.00 | 0.016 | 1.00 | 0.67 |

3.86.9 Detailed Probabilities of LYS86HB3:

Overall probability: 0.962

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS86 | 0.95 | 1.00 |
| PRO87 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K86HA | 1.00 |
| K86HB2 | 1.00 |
| K86HG2 | 1.00 |
| K86HG3 | 1.00 |
| K86HD2 | 1.00 |
| K86HD3 | 1.00 |
| K86HE2 | 0.99 |
| K86HE3 | 0.99 |
| K86H | 1.00 |
| K86HB3 | 1.00 |
| P87HD2 | 0.99 |
| P87HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS86 | HA | 1.00 | 0.001 | 1.00 | 0.76 |
| LYS86 | HB2 | 1.00 | 0.003 | 1.00 | 1.38 |
| LYS86 | HB3 | 1.00 | 0.012 | 1.00 | 29.96 |
| LYS86 | HG2 | 1.00 | 0.007 | 1.00 | 1.71 |
| LYS86 | HG3 | 1.00 | 0.035 | 0.50 | 0.00 |
| LYS86 | HD2 | 1.00 | 0.002 | 1.00 | 1.24 |
| LYS86 | HD3 | 1.00 | 0.002 | 1.00 | 1.24 |
| LYS86 | HE2 | 0.99 | 0.001 | 1.00 | 0.45 |
| LYS86 | HE3 | 0.99 | 0.001 | 1.00 | 0.45 |
| LYS86 | H | 1.00 | 0.001 | 1.00 | -2185740.00 |
| PRO87 | HD2 | 0.99 | 0.005 | 1.00 | 1.33 |
| PRO87 | HD3 | 1.00 | 0.002 | 1.00 | 1.13 |
| PRO87 | HG2 | 0.53 | 0.006 | 1.00 | 18.77 |

3.86.10 Detailed Probabilities of LYS86HG2:

Overall probability: 0.900

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS86 | 0.90 | 0.91 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K86HA | 1.00 |
| K86HB2 | 1.00 |
| K86HB3 | 1.00 |
| K86HG3 | 1.00 |
| K86HD2 | 1.00 |
| K86HD3 | 1.00 |
| K86HE2 | 1.00 |
| K86HE3 | 1.00 |
| K86H | 1.00 |
| K86HZ2 | 1.00 |
| K86HG2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS86 | HA | 1.00 | 0.005 | 1.00 | 0.46 |
| LYS86 | HB2 | 1.00 | 0.005 | 1.00 | 0.24 |
| LYS86 | HB3 | 1.00 | 0.015 | 1.00 | 0.86 |
| LYS86 | HG2 | 1.00 | 0.018 | 1.00 | 10.96 |
| LYS86 | HG3 | 1.00 | 0.002 | 1.00 | 1.30 |
| LYS86 | HD2 | 1.00 | 0.002 | 1.00 | 0.66 |
| LYS86 | HD3 | 1.00 | 0.002 | 1.00 | 0.66 |
| LYS86 | HE2 | 1.00 | 0.451 | 0.00 | 0.00 |
| LYS86 | HE3 | 1.00 | 0.016 | 1.00 | 0.58 |
| LYS86 | H | 1.00 | 0.002 | 1.00 | -370801.00 |

3.86.11 Detailed Probabilities of LYS86HG3:

Overall probability: 0.950

Overall confidence: 0.909

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS86 | 0.95 | 0.91 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K86HA | 1.00 |
| K86HB2 | 1.00 |
| K86HB3 | 1.00 |
| K86HG2 | 1.00 |
| K86HD2 | 1.00 |
| K86HD3 | 1.00 |
| K86HE2 | 1.00 |
| K86HE3 | 1.00 |
| K86H | 1.00 |
| K86HZ2 | 1.00 |
| K86HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS86 | HA | 1.00 | 0.001 | 1.00 | 0.76 |
| LYS86 | HB2 | 1.00 | 0.003 | 1.00 | 1.38 |
| LYS86 | HB3 | 1.00 | 0.012 | 1.00 | 29.96 |
| LYS86 | HG2 | 1.00 | 0.007 | 1.00 | 1.71 |
| LYS86 | HG3 | 1.00 | 0.035 | 0.50 | 0.00 |
| LYS86 | HD2 | 1.00 | 0.002 | 1.00 | 1.24 |
| LYS86 | HD3 | 1.00 | 0.002 | 1.00 | 1.24 |
| LYS86 | HE2 | 1.00 | 0.001 | 1.00 | 0.45 |
| LYS86 | HE3 | 1.00 | 0.001 | 1.00 | 0.45 |
| LYS86 | H | 1.00 | 0.001 | 1.00 | -2185740.00 |

3.86.12 Detailed Probabilities of LYS86HD2:

Overall probability: 0.602

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS86 | 0.60 | 0.90 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K86HA | 0.98 |
| K86HB2 | 1.00 |
| K86HB3 | 1.00 |
| K86HG2 | 1.00 |
| K86HG3 | 1.00 |
| K86HD3 | 1.00 |
| K86HE2 | 1.00 |
| K86HE3 | 1.00 |
| K86HZ2 | 1.00 |
| K86HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS86 | HA | 0.98 | 0.043 | 0.02 | 0.00 |
| LYS86 | HB2 | 1.00 | 0.259 | 0.00 | 0.00 |
| LYS86 | HB3 | 1.00 | 0.044 | 0.00 | 0.00 |
| LYS86 | HG2 | 1.00 | 0.083 | 0.00 | 0.00 |
| LYS86 | HG3 | 1.00 | 0.020 | 1.00 | 3.12 |
| LYS86 | HD2 | 1.00 | 0.001 | 1.00 | 20.46 |
| LYS86 | HD3 | 1.00 | 0.001 | 1.00 | 20.46 |
| LYS86 | HE2 | 1.00 | 0.003 | 1.00 | 0.87 |
| LYS86 | HE3 | 1.00 | 0.003 | 1.00 | 0.87 |
| LYS86 | H | 0.88 | 0.008 | 1.00 | -988804.00 |

3.86.13 Detailed Probabilities of LYS86HD3:

Overall probability: 0.602

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS86 | 0.60 | 0.90 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K86HA | 0.98 |
| K86HB2 | 1.00 |
| K86HB3 | 1.00 |
| K86HG2 | 1.00 |
| K86HG3 | 1.00 |
| K86HD2 | 1.00 |
| K86HE2 | 1.00 |
| K86HE3 | 1.00 |
| K86HZ2 | 1.00 |
| K86HD3 | 1.00 |

NOESY contacts detailed probability

3.86 LYS(86)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS86 | HA | 0.98 | 0.045 | 0.02 | 0.00 |
| LYS86 | HB2 | 1.00 | 0.261 | 0.00 | 0.00 |
| LYS86 | HB3 | 1.00 | 0.046 | 0.00 | 0.00 |
| LYS86 | HG2 | 1.00 | 0.085 | 0.00 | 0.00 |
| LYS86 | HG3 | 1.00 | 0.018 | 1.00 | 3.12 |
| LYS86 | HD2 | 1.00 | 0.003 | 1.00 | 20.46 |
| LYS86 | HD3 | 1.00 | 0.003 | 1.00 | 20.46 |
| LYS86 | HE2 | 1.00 | 0.001 | 1.00 | 0.87 |
| LYS86 | HE3 | 1.00 | 0.001 | 1.00 | 0.87 |
| LYS86 | H | 0.87 | 0.006 | 1.00 | -988804.00 |

3.86.14 Detailed Probabilities of LYS86HE2:

Overall probability: 0.791

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS86 | 0.79 | 0.89 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K86HB2 | 0.98 |
| K86HB3 | 0.99 |
| K86HG2 | 1.00 |
| K86HG3 | 1.00 |
| K86HD2 | 1.00 |
| K86HD3 | 1.00 |
| K86HE3 | 1.00 |
| K86HZ2 | 1.00 |
| K86HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS86 | HB2 | 0.98 | 0.642 | 0.02 | 0.00 |
| LYS86 | HB3 | 0.99 | 0.022 | 1.00 | 0.11 |
| LYS86 | HG2 | 1.00 | 0.025 | 1.00 | 0.15 |
| LYS86 | HG3 | 1.00 | 0.023 | 1.00 | 0.25 |
| LYS86 | HD2 | 1.00 | 0.023 | 1.00 | 0.79 |
| LYS86 | HD3 | 1.00 | 0.023 | 1.00 | 0.79 |
| LYS86 | HE2 | 1.00 | 0.007 | 1.00 | 14.74 |
| LYS86 | HE3 | 1.00 | 0.039 | 0.10 | 0.00 |
| LYS86 | HA | 0.77 | 0.019 | 1.00 | 0.05 |

3.86.15 Detailed Probabilities of LYS86HE3:

Overall probability: 0.890

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS86 | 0.89 | 0.89 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K86HB2 | 0.99 |
| K86HB3 | 0.99 |
| K86HG2 | 1.00 |
| K86HG3 | 1.00 |
| K86HD2 | 1.00 |
| K86HD3 | 1.00 |
| K86HE2 | 1.00 |
| K86HZ2 | 1.00 |
| K86HE3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS86 | HB2 | 0.99 | 0.676 | 0.01 | 0.00 |
| LYS86 | HB3 | 0.99 | 0.012 | 1.00 | 0.11 |
| LYS86 | HG2 | 1.00 | 0.009 | 1.00 | 0.15 |
| LYS86 | HG3 | 1.00 | 0.011 | 1.00 | 0.25 |
| LYS86 | HD2 | 1.00 | 0.011 | 1.00 | 0.79 |
| LYS86 | HD3 | 1.00 | 0.011 | 1.00 | 0.79 |
| LYS86 | HE2 | 1.00 | 0.027 | 1.00 | 14.74 |
| LYS86 | HE3 | 1.00 | 0.005 | 1.00 | 25.44 |
| LYS86 | HA | 0.76 | 0.015 | 1.00 | 0.05 |

3.86.16 Detailed Probabilities of LYS86H:

Overall probability: 0.867

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU85 | 0.83 | 1.00 |
| LYS86 | 0.83 | 1.00 |
| PRO87 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| L85HA | 1.00 |
| L85H | 1.00 |
| L85HB3 | 1.00 |
| L85HB2 | 1.00 |
| L85HG | 0.98 |
| K86HA | 1.00 |
| K86HB2 | 1.00 |
| K86HB3 | 1.00 |
| K86HG2 | 1.00 |
| K86HG3 | 1.00 |
| K86H | 1.00 |
| P87HD2 | 0.99 |
| P87HD3 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU85 | HA | 1.00 | 0.225 | 0.00 | 0.00 |
| LEU85 | HB2 | 1.00 | 0.003 | 1.00 | 0.17 |
| LEU85 | HB3 | 1.00 | 0.000 | 1.00 | 0.21 |
| LEU85 | HG | 0.98 | 0.003 | 1.00 | 0.22 |
| LEU85 | H | 1.00 | 0.001 | 1.00 | -2656679.00 |
| LEU85 | HD21 | 0.59 | 0.003 | 1.00 | 0.29 |
| LYS86 | HA | 1.00 | 0.005 | 1.00 | 0.40 |
| LYS86 | HB2 | 1.00 | 1.240 | 0.00 | 0.00 |
| LYS86 | HB3 | 1.00 | 0.007 | 1.00 | 0.33 |
| LYS86 | HG2 | 1.00 | 0.001 | 1.00 | 0.14 |
| LYS86 | HG3 | 1.00 | 0.003 | 1.00 | 0.29 |
| LYS86 | H | 1.00 | 0.001 | 1.00 | -8587671.00 |
| PRO87 | HD2 | 0.99 | 0.002 | 1.00 | 0.39 |
| PRO87 | HD3 | 0.99 | 0.002 | 1.00 | 0.40 |
| PRO87 | HA | 0.68 | 0.005 | 1.00 | 0.07 |

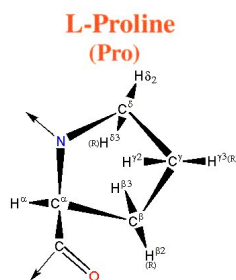
3.87 PRO(87)

Figure 77: Image from the BMRB

Residue probability: 0.648

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 179.579 | 175.173 | 13.901 | 0.000 | 0.000 |
| CA 3.87.1 | 66.718 | 62.931 | 15.301 | 0.654 | 1.000 |
| CB 3.87.2 | 30.461 | 33.632 | 13.629 | 0.375 | 1.000 |
| CG 3.87.3 | 28.529 | 28.412 | 13.801 | 0.857 | 1.000 |
| CD 3.87.4 | 50.193 | 49.797 | 3.175 | 0.923 | 1.000 |
| N | NA | - | - | 0.000 | 0.000 |
| HA 3.87.5 | 4.287 | 4.332 | 0.427 | 0.700 | 1.000 |
| HB2 3.87.6 | 1.914 | 2.099 | 0.501 | 0.268 | 1.000 |
| HB3 3.87.7 | 2.360 | 2.052 | 0.596 | 0.625 | 1.000 |
| HG2 3.87.8 | 1.970 | 1.927 | 0.364 | 0.571 | 1.000 |
| HG3 3.87.9 | 2.184 | 1.907 | 0.417 | 0.643 | 1.000 |
| HD2 3.87.10 | 3.657 | 3.640 | 0.682 | 0.786 | 1.000 |
| HD3 3.87.11 | 3.449 | 3.558 | 0.522 | 0.727 | 1.000 |

3.87.1 Detailed Probabilities of PRO87CA:

Overall probability: 0.654

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS86 | 0.63 | 1.00 |
| PRO87 | 0.86 | 1.00 |
| ASP88 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K86HA | 1.00 |
| P87HB2 | 1.00 |
| P87HB3 | 1.00 |
| P87HG2 | 1.00 |
| P87HG3 | 1.00 |
| P87HD2 | 1.00 |
| P87HD3 | 1.00 |
| P87HA | 1.00 |
| D88H | 1.00 |
| D88HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS86 | HA | 1.00 | 0.130 | 0.00 | 0.00 |
| LYS86 | HB2 | 0.58 | 0.033 | 0.70 | 0.00 |
| LYS86 | HB3 | 0.80 | 0.032 | 0.80 | 0.00 |
| LYS86 | H | 0.68 | 0.005 | 1.00 | 0.07 |
| PRO87 | HA | 1.00 | 0.000 | 1.00 | 4.95 |
| PRO87 | HB2 | 1.00 | 0.016 | 1.00 | 0.59 |
| PRO87 | HB3 | 1.00 | 0.003 | 1.00 | 0.78 |
| PRO87 | HG2 | 1.00 | 0.040 | 0.00 | 0.00 |
| PRO87 | HG3 | 1.00 | 0.001 | 1.00 | 0.22 |
| PRO87 | HD2 | 1.00 | 0.017 | 1.00 | 0.11 |
| PRO87 | HD3 | 1.00 | 0.013 | 1.00 | 0.09 |
| ASP88 | HA | 1.00 | 0.330 | 0.00 | 0.00 |
| ASP88 | H | 1.00 | 0.086 | 0.00 | 0.00 |

3.87.2 Detailed Probabilities of PRO87CB:

Overall probability: 0.375

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO87 | 0.29 | 1.00 |
| ASP88 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P87HA | 1.00 |
| P87HB2 | 1.00 |
| P87HG2 | 1.00 |
| P87HG3 | 1.00 |
| P87HD2 | 1.00 |
| P87HD3 | 1.00 |
| P87HB3 | 1.00 |
| D88H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO87 | HA | 1.00 | 0.002 | 1.00 | 0.76 |
| PRO87 | HB2 | 1.00 | 1.740 | 0.00 | 0.00 |
| PRO87 | HB3 | 1.00 | 1.294 | 0.00 | 0.00 |
| PRO87 | HG2 | 1.00 | 1.684 | 0.00 | 0.00 |
| PRO87 | HG3 | 1.00 | 1.470 | 0.00 | 0.00 |
| PRO87 | HD2 | 1.00 | 0.003 | 1.00 | 0.18 |
| PRO87 | HD3 | 1.00 | 0.205 | 0.00 | 0.00 |
| ASP88 | H | 1.00 | 0.007 | 1.00 | 0.27 |

3.87.3 Detailed Probabilities of PRO87CG:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO87 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P87HA | 1.00 |
| P87HB2 | 1.00 |
| P87HB3 | 1.00 |
| P87HG2 | 1.00 |
| P87HD2 | 1.00 |
| P87HD3 | 1.00 |
| P87HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO87 | HA | 1.00 | 0.007 | 1.00 | 0.25 |
| PRO87 | HB2 | 1.00 | 0.048 | 0.00 | 0.00 |
| PRO87 | HB3 | 1.00 | 0.002 | 1.00 | 0.79 |
| PRO87 | HG2 | 1.00 | 0.008 | 1.00 | 2.62 |
| PRO87 | HG3 | 1.00 | 0.004 | 1.00 | 4.03 |
| PRO87 | HD2 | 1.00 | 0.005 | 1.00 | 0.62 |
| PRO87 | HD3 | 1.00 | 0.001 | 1.00 | 0.63 |

3.87.4 Detailed Probabilities of PRO87CD:

Overall probability: 0.923

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS86 | 1.00 | 1.00 |
| PRO87 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K86HB3 | 1.00 |
| K86HA | 1.00 |
| K86HB2 | 1.00 |
| K86H | 0.99 |
| P87HA | 1.00 |
| P87HB2 | 1.00 |
| P87HB3 | 1.00 |
| P87HG2 | 1.00 |
| P87HG3 | 1.00 |
| P87HD2 | 1.00 |
| P87HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS86 | HA | 1.00 | 0.026 | 1.00 | 0.27 |
| LYS86 | HB2 | 1.00 | 0.016 | 1.00 | 0.67 |
| LYS86 | HB3 | 1.00 | 0.002 | 1.00 | 1.13 |
| LYS86 | H | 0.99 | 0.002 | 1.00 | 0.40 |
| LYS86 | HG2 | 0.79 | 0.006 | 1.00 | 0.08 |
| LYS86 | HG3 | 0.78 | 0.002 | 1.00 | 1.13 |
| PRO87 | HA | 1.00 | 0.003 | 1.00 | 0.13 |
| PRO87 | HB2 | 1.00 | 0.050 | 0.00 | 0.00 |
| PRO87 | HB3 | 1.00 | 0.002 | 1.00 | 0.20 |
| PRO87 | HG2 | 1.00 | 0.006 | 1.00 | 1.13 |
| PRO87 | HG3 | 1.00 | 0.007 | 1.00 | 0.73 |
| PRO87 | HD2 | 1.00 | 0.000 | 1.00 | 3.70 |
| PRO87 | HD3 | 1.00 | 0.010 | 1.00 | 5.16 |

3.87.5 Detailed Probabilities of PRO87HA:

Overall probability: 0.700

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS86 | 0.00 | 1.00 |
| PRO87 | 0.71 | 1.00 |
| ASP88 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K86HA | 1.00 |
| P87HB2 | 1.00 |
| P87HB3 | 1.00 |
| P87HG2 | 1.00 |
| P87HG3 | 1.00 |
| P87HD2 | 1.00 |
| P87HD3 | 1.00 |
| P87HA | 1.00 |
| D88H | 1.00 |
| D88HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS86 | HA | 1.00 | 0.311 | 0.00 | 0.00 |
| PRO87 | HA | 1.00 | 0.000 | 1.00 | 4.95 |
| PRO87 | HB2 | 1.00 | 0.068 | 0.00 | 0.00 |
| PRO87 | HB3 | 1.00 | 0.002 | 1.00 | 0.76 |
| PRO87 | HG2 | 1.00 | 2.065 | 0.00 | 0.00 |
| PRO87 | HG3 | 1.00 | 0.007 | 1.00 | 0.25 |
| PRO87 | HD2 | 1.00 | 0.001 | 1.00 | 0.12 |
| PRO87 | HD3 | 1.00 | 0.003 | 1.00 | 0.13 |
| ASP88 | HA | 1.00 | 0.015 | 1.00 | 0.14 |
| ASP88 | H | 1.00 | 0.002 | 1.00 | -300985.00 |

3.87.6 Detailed Probabilities of PRO87HB2:

Overall probability: 0.268

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO87 | 0.20 | 1.00 |
| ASP88 | 0.51 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P87HA | 1.00 |
| P87HB3 | 1.00 |
| P87HG2 | 1.00 |
| P87HG3 | 1.00 |
| P87HD2 | 1.00 |
| P87HD3 | 1.00 |
| P87HB2 | 1.00 |
| D88HA | 0.99 |
| D88H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO87 | HA | 1.00 | 0.016 | 1.00 | 0.59 |
| PRO87 | HB2 | 1.00 | 0.111 | 0.00 | 0.00 |
| PRO87 | HB3 | 1.00 | 1.740 | 0.00 | 0.00 |
| PRO87 | HG2 | 1.00 | 0.036 | 0.40 | 0.00 |
| PRO87 | HG3 | 1.00 | 0.048 | 0.00 | 0.00 |
| PRO87 | HD2 | 1.00 | 0.053 | 0.00 | 0.00 |
| PRO87 | HD3 | 1.00 | 0.050 | 0.00 | 0.00 |
| ASP88 | HA | 0.99 | 0.052 | 0.01 | 0.00 |
| ASP88 | H | 1.00 | 0.003 | 1.00 | -1004488.00 |

3.87.7 Detailed Probabilities of PRO87HB3:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO87 | 0.57 | 1.00 |
| ASP88 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P87HA | 1.00 |
| P87HB2 | 1.00 |
| P87HG2 | 1.00 |
| P87HG3 | 1.00 |
| P87HD2 | 1.00 |
| P87HD3 | 1.00 |
| P87HB3 | 1.00 |
| D88H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO87 | HA | 1.00 | 0.003 | 1.00 | 0.78 |
| PRO87 | HB2 | 1.00 | 0.557 | 0.00 | 0.00 |
| PRO87 | HB3 | 1.00 | 1.294 | 0.00 | 0.00 |
| PRO87 | HG2 | 1.00 | 0.138 | 0.00 | 0.00 |
| PRO87 | HG3 | 1.00 | 0.002 | 1.00 | 0.79 |
| PRO87 | HD2 | 1.00 | 0.002 | 1.00 | 0.12 |
| PRO87 | HD3 | 1.00 | 0.002 | 1.00 | 0.20 |
| ASP88 | H | 1.00 | 0.005 | 1.00 | -452100.00 |

3.87.8 Detailed Probabilities of PRO87HG2:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO87 | 0.57 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P87HA | 1.00 |
| P87HB2 | 1.00 |
| P87HB3 | 1.00 |
| P87HG3 | 1.00 |
| P87HD2 | 1.00 |
| P87HD3 | 1.00 |
| P87HG2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO87 | HA | 1.00 | 0.040 | 0.00 | 0.00 |
| PRO87 | HB2 | 1.00 | 0.167 | 0.00 | 0.00 |
| PRO87 | HB3 | 1.00 | 1.684 | 0.00 | 0.00 |
| PRO87 | HG2 | 1.00 | 0.014 | 1.00 | 18.77 |
| PRO87 | HG3 | 1.00 | 0.008 | 1.00 | 2.62 |
| PRO87 | HD2 | 1.00 | 0.003 | 1.00 | 1.33 |
| PRO87 | HD3 | 1.00 | 0.006 | 1.00 | 1.13 |

3.87.9 Detailed Probabilities of PRO87HG3:

Overall probability: 0.643

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO87 | 0.64 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P87HA | 1.00 |
| P87HB2 | 1.00 |
| P87HB3 | 1.00 |
| P87HG2 | 1.00 |
| P87HD2 | 1.00 |
| P87HD3 | 1.00 |
| P87HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO87 | HA | 1.00 | 0.001 | 1.00 | 0.22 |
| PRO87 | HB2 | 1.00 | 0.381 | 0.00 | 0.00 |
| PRO87 | HB3 | 1.00 | 1.470 | 0.00 | 0.00 |
| PRO87 | HG2 | 1.00 | 0.035 | 0.50 | 0.00 |
| PRO87 | HG3 | 1.00 | 0.004 | 1.00 | 4.03 |
| PRO87 | HD2 | 1.00 | 0.007 | 1.00 | 0.52 |
| PRO87 | HD3 | 1.00 | 0.007 | 1.00 | 0.73 |

3.87.10 Detailed Probabilities of PRO87HD2:

Overall probability: 0.786

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS86 | 0.86 | 1.00 |
| PRO87 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K86H | 0.99 |
| K86HB3 | 0.99 |
| K86HA | 1.00 |
| K86HB2 | 0.99 |
| P87HA | 1.00 |
| P87HB2 | 1.00 |
| P87HB3 | 1.00 |
| P87HG2 | 1.00 |
| P87HG3 | 1.00 |
| P87HD3 | 1.00 |
| P87HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS86 | HA | 1.00 | 0.045 | 0.00 | 0.00 |
| LYS86 | HB2 | 0.99 | 0.000 | 1.00 | 0.26 |
| LYS86 | HB3 | 0.99 | 0.003 | 1.00 | 0.35 |
| LYS86 | H | 0.99 | 0.005 | 1.00 | -717663.00 |
| LYS86 | HG2 | 0.93 | 0.029 | 1.00 | 0.16 |
| LYS86 | HD2 | 0.66 | 0.003 | 1.00 | 0.14 |
| LYS86 | HD3 | 0.66 | 0.003 | 1.00 | 0.14 |
| PRO87 | HA | 1.00 | 0.017 | 1.00 | 0.11 |
| PRO87 | HB2 | 1.00 | 0.146 | 0.00 | 0.00 |
| PRO87 | HB3 | 1.00 | 0.003 | 1.00 | 0.18 |
| PRO87 | HG2 | 1.00 | 1.435 | 0.00 | 0.00 |
| PRO87 | HG3 | 1.00 | 0.005 | 1.00 | 0.62 |
| PRO87 | HD2 | 1.00 | 0.000 | 1.00 | 5.13 |
| PRO87 | HD3 | 1.00 | 0.000 | 1.00 | 3.70 |

3.87.11 Detailed Probabilities of PRO87HD3:

Overall probability: 0.727

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LYS86 | 1.00 | 1.00 |
| PRO87 | 0.57 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| K86HB3 | 1.00 |
| K86HA | 1.00 |
| K86HB2 | 1.00 |
| K86H | 0.99 |
| P87HA | 1.00 |
| P87HB2 | 1.00 |
| P87HB3 | 1.00 |
| P87HG2 | 1.00 |
| P87HG3 | 1.00 |
| P87HD2 | 1.00 |
| P87HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LYS86 | HA | 1.00 | 0.000 | 1.00 | 0.05 |
| LYS86 | HB2 | 1.00 | 0.005 | 1.00 | 0.13 |
| LYS86 | HB3 | 1.00 | 0.002 | 1.00 | 0.22 |
| LYS86 | H | 0.99 | 0.004 | 1.00 | -587899.00 |
| PRO87 | HA | 1.00 | 0.013 | 1.00 | 0.09 |
| PRO87 | HB2 | 1.00 | 0.336 | 0.00 | 0.00 |
| PRO87 | HB3 | 1.00 | 0.205 | 0.00 | 0.00 |
| PRO87 | HG2 | 1.00 | 1.227 | 0.00 | 0.00 |
| PRO87 | HG3 | 1.00 | 0.001 | 1.00 | 0.63 |
| PRO87 | HD2 | 1.00 | 0.010 | 1.00 | 3.77 |
| PRO87 | HD3 | 1.00 | 0.010 | 1.00 | 5.16 |

3.88 ASP(88)

Figure 78: Image from the BMRB

Residue probability: 0.781

Residue probability confidence: 0.897

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 179.137 | 176.463 | 2.348 | 0.000 | 0.000 |
| CA 3.88.1 | 57.146 | 54.786 | 4.266 | 0.701 | 0.889 |
| CB 3.88.2 | 40.867 | 40.949 | 3.070 | 0.800 | 0.833 |
| N 3.88.3 | 116.681 | 120.550 | 5.690 | 1.000 | 1.000 |
| HD2 | NA | – | – | 0.000 | 0.000 |
| HA 3.88.4 | 4.617 | 4.587 | 0.329 | 0.502 | 0.889 |
| HB2 3.88.5 | 2.679 | 2.708 | 0.282 | 0.833 | 0.833 |
| HB3 3.88.6 | 2.591 | 2.654 | 0.285 | 0.800 | 0.833 |
| H 3.88.7 | 7.457 | 8.304 | 1.027 | 0.833 | 1.000 |

3.88.1 Detailed Probabilities of ASP88CA:

Overall probability: 0.701

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO87 | 0.67 | 1.00 |
| ASP88 | 0.75 | 0.80 |
| ILE89 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P87HA | 1.00 |
| P87HB2 | 0.99 |
| D88HD2 | 1.00 |
| D88HB2 | 1.00 |
| D88HB3 | 1.00 |
| D88H | 1.00 |
| D88HA | 1.00 |
| I89H | 1.00 |
| I89HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO87 | HA | 1.00 | 0.015 | 1.00 | 0.14 |
| PRO87 | HB2 | 0.99 | 0.052 | 0.01 | 0.00 |
| PRO87 | HG2 | 0.63 | 0.004 | 1.00 | 0.23 |
| ASP88 | HA | 1.00 | 0.101 | 0.00 | 0.00 |
| ASP88 | HB2 | 1.00 | 0.010 | 1.00 | 0.58 |
| ASP88 | HB3 | 1.00 | 0.007 | 1.00 | 0.83 |
| ASP88 | H | 1.00 | 0.010 | 1.00 | 1.09 |
| ILE89 | HA | 1.00 | 0.195 | 0.00 | 0.00 |
| ILE89 | H | 1.00 | 0.008 | 1.00 | 0.28 |
| ILE89 | HG13 | 0.62 | 0.001 | 1.00 | 0.07 |

3.88.2 Detailed Probabilities of ASP88CB:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP88 | 0.75 | 0.80 |
| ILE89 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D88HD2 | 1.00 |
| D88HA | 1.00 |
| D88HB3 | 1.00 |
| D88H | 1.00 |
| D88HB2 | 1.00 |
| I89H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP88 | HA | 1.00 | 0.003 | 1.00 | 1.43 |
| ASP88 | HB2 | 1.00 | 0.095 | 0.00 | 0.00 |
| ASP88 | HB3 | 1.00 | 0.007 | 1.00 | 2.55 |
| ASP88 | H | 1.00 | 0.005 | 1.00 | 0.59 |
| ILE89 | H | 1.00 | 0.013 | 1.00 | 0.21 |

3.88.3 Detailed Probabilities of ASP88N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO87 | 1.00 | 1.00 |
| ASP88 | 1.00 | 1.00 |
| ILE89 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P87HB2 | 1.00 |
| P87HB3 | 1.00 |
| P87HA | 1.00 |
| D88HA | 1.00 |
| D88HB2 | 1.00 |
| D88HB3 | 1.00 |
| D88H | 1.00 |
| I89H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO87 | HA | 1.00 | 0.002 | 1.00 | -300985.00 |
| PRO87 | HB2 | 1.00 | 0.003 | 1.00 | -1004488.00 |
| PRO87 | HB3 | 1.00 | 0.005 | 1.00 | -452100.00 |
| PRO87 | HG3 | 0.87 | 0.001 | 1.00 | -280283.00 |
| PRO87 | HD2 | 0.82 | 0.004 | 1.00 | -269386.00 |
| PRO87 | HD3 | 0.72 | 0.005 | 1.00 | -601947.00 |
| ASP88 | HA | 1.00 | 0.003 | 1.00 | -1368172.00 |
| ASP88 | HB2 | 1.00 | 0.006 | 1.00 | -1700870.00 |
| ASP88 | HB3 | 1.00 | 0.005 | 1.00 | -1187462.00 |
| ASP88 | H | 1.00 | 0.006 | 1.00 | -13213099.00 |
| ILE89 | H | 1.00 | 0.006 | 1.00 | -1636305.00 |
| ILE89 | HA | 0.91 | 0.001 | 1.00 | -113360.00 |
| ILE89 | HB | 0.52 | 0.009 | 1.00 | -137511.00 |
| ILE89 | HG13 | 0.56 | 0.010 | 1.00 | -115654.00 |

3.88.4 Detailed Probabilities of ASP88HA:

Overall probability: 0.502

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO87 | 0.01 | 1.00 |
| ASP88 | 0.75 | 0.80 |
| ILE89 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P87HA | 1.00 |
| P87HB2 | 0.99 |
| D88HD2 | 1.00 |
| D88HB2 | 1.00 |
| D88HB3 | 1.00 |
| D88H | 1.00 |
| D88HA | 1.00 |
| I89H | 1.00 |
| I89HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO87 | HA | 1.00 | 0.330 | 0.00 | 0.00 |
| PRO87 | HB2 | 0.99 | 0.206 | 0.01 | 0.00 |
| ASP88 | HA | 1.00 | 0.101 | 0.00 | 0.00 |
| ASP88 | HB2 | 1.00 | 0.003 | 1.00 | 1.43 |
| ASP88 | HB3 | 1.00 | 0.000 | 1.00 | 0.67 |
| ASP88 | H | 1.00 | 0.003 | 1.00 | -1368172.00 |
| ILE89 | HA | 1.00 | 0.296 | 0.00 | 0.00 |
| ILE89 | H | 1.00 | 0.005 | 1.00 | -327917.00 |

3.88.5 Detailed Probabilities of ASP88HB2:

Overall probability: 0.833

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP88 | 0.75 | 0.80 |
| ILE89 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D88HD2 | 1.00 |
| D88HA | 1.00 |
| D88HB3 | 1.00 |
| D88H | 1.00 |
| D88HB2 | 1.00 |
| I89H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP88 | HA | 1.00 | 0.010 | 1.00 | 0.58 |
| ASP88 | HB2 | 1.00 | 0.095 | 0.00 | 0.00 |
| ASP88 | HB3 | 1.00 | 0.008 | 1.00 | 2.42 |
| ASP88 | H | 1.00 | 0.006 | 1.00 | -1700870.00 |
| ILE89 | H | 1.00 | 0.005 | 1.00 | -393719.00 |
| ILE89 | HA | 0.59 | 0.006 | 1.00 | 0.05 |

3.88.6 Detailed Probabilities of ASP88HB3:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP88 | 0.75 | 0.80 |
| ILE89 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D88HD2 | 1.00 |
| D88HA | 1.00 |
| D88HB2 | 1.00 |
| D88H | 1.00 |
| D88HB3 | 1.00 |
| I89H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP88 | HA | 1.00 | 0.007 | 1.00 | 0.83 |
| ASP88 | HB2 | 1.00 | 0.007 | 1.00 | 2.55 |
| ASP88 | HB3 | 1.00 | 0.080 | 0.00 | 0.00 |
| ASP88 | H | 1.00 | 0.005 | 1.00 | -1187462.00 |
| ILE89 | H | 1.00 | 0.005 | 1.00 | -263018.00 |

3.88.7 Detailed Probabilities of ASP88H:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO87 | 0.71 | 1.00 |
| ASP88 | 1.00 | 1.00 |
| ILE89 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| P87HB2 | 1.00 |
| P87HB3 | 1.00 |
| P87HA | 1.00 |
| D88HA | 1.00 |
| D88HB2 | 1.00 |
| D88HB3 | 1.00 |
| D88H | 1.00 |
| I89H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO87 | HA | 1.00 | 0.086 | 0.00 | 0.00 |
| PRO87 | HB2 | 1.00 | 0.042 | 0.00 | 0.00 |
| PRO87 | HB3 | 1.00 | 0.007 | 1.00 | 0.27 |
| PRO87 | HG2 | 0.95 | 0.015 | 1.00 | 0.12 |
| PRO87 | HG3 | 0.87 | 0.006 | 1.00 | 0.19 |
| PRO87 | HD2 | 0.82 | 0.020 | 1.00 | 0.22 |
| PRO87 | HD3 | 0.72 | 0.012 | 1.00 | 0.38 |
| ASP88 | HA | 1.00 | 0.010 | 1.00 | 1.09 |
| ASP88 | HB2 | 1.00 | 0.005 | 1.00 | 0.59 |
| ASP88 | HB3 | 1.00 | 0.006 | 1.00 | 0.53 |
| ASP88 | H | 1.00 | 0.006 | 1.00 | -13213099.00 |
| ILE89 | H | 1.00 | 0.006 | 1.00 | -1137509.00 |

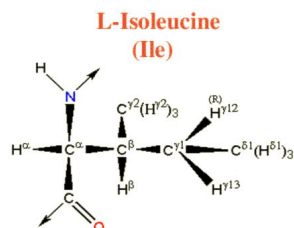
3.89 ILE(89)

Figure 79: Image from the BMRB

Residue probability: 0.897

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|--------------|-------------|---------|--------|---------------------|--------------------|
| C | 177.213 | 175.926 | 2.710 | 0.000 | 0.000 |
| CA 3.89.1 | 65.923 | 61.717 | 4.152 | 0.909 | 1.000 |
| CB 3.89.2 | 37.729 | 38.702 | 3.945 | 0.778 | 1.000 |
| CG1 3.89.3 | 29.383 | 27.785 | 2.037 | 1.000 | 1.000 |
| CG2 3.89.4 | 16.176 | 17.574 | 1.928 | 1.000 | 1.000 |
| CD1 3.89.5 | 15.665 | 13.545 | 3.646 | 0.857 | 1.000 |
| N 3.89.6 | 124.521 | 121.467 | 6.098 | 1.000 | 1.000 |
| HA 3.89.7 | 3.207 | 4.185 | 1.403 | 0.727 | 1.000 |
| HB 3.89.8 | 1.452 | 1.776 | 0.310 | 0.778 | 1.000 |
| HG12 3.89.9 | 1.830 | 1.271 | 0.411 | 0.750 | 1.000 |
| HG13 3.89.10 | 0.582 | 1.186 | 0.426 | 1.000 | 1.000 |
| HG2 3.89.11 | -0.220 | 0.762 | 0.283 | 1.000 | 1.000 |
| HD1 3.89.12 | 0.861 | 0.668 | 0.293 | 0.857 | 1.000 |
| H 3.89.13 | 8.154 | 8.301 | 0.685 | 1.000 | 1.000 |

3.89.1 Detailed Probabilities of ILE89CA:

Overall probability: 0.909

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP88 | 0.50 | 1.00 |
| ILE89 | 1.00 | 1.00 |
| TYR90 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| D88HA | 1.00 |
| I89HB | 1.00 |
| I89HG12 | 1.00 |
| I89HG13 | 1.00 |
| I89HG21 | 1.00 |
| I89HD11 | 0.97 |
| I89H | 1.00 |
| I89HA | 1.00 |
| Y90HA | 1.00 |
| Y90H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP88 | HA | 1.00 | 0.296 | 0.00 | 0.00 |
| ASP88 | HB2 | 0.59 | 0.006 | 1.00 | 0.05 |
| ILE89 | HA | 1.00 | 0.002 | 1.00 | 5.18 |
| ILE89 | HB | 1.00 | 0.001 | 1.00 | 0.26 |
| ILE89 | HG12 | 1.00 | 0.000 | 1.00 | 0.49 |
| ILE89 | HG13 | 1.00 | 0.005 | 1.00 | 0.62 |
| ILE89 | HG21 | 1.00 | 0.000 | 1.00 | 0.77 |
| ILE89 | HD11 | 0.97 | 0.002 | 1.00 | 0.47 |
| ILE89 | H | 1.00 | 0.003 | 1.00 | 0.40 |
| TYR90 | HA | 1.00 | 0.021 | 1.00 | 0.12 |
| TYR90 | H | 1.00 | 0.003 | 1.00 | 0.11 |

3.89.2 Detailed Probabilities of ILE89CB:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE89 | 0.71 | 1.00 |
| TYR90 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I89HA | 1.00 |
| I89HG12 | 1.00 |
| I89HG13 | 1.00 |
| I89HG21 | 1.00 |
| I89HD11 | 1.00 |
| I89H | 1.00 |
| I89HB | 1.00 |
| Y90H | 1.00 |

NOESY contacts detailed probability

3.89 ILE(89)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE89 | HA | 1.00 | 0.000 | 1.00 | 0.40 |
| ILE89 | HB | 1.00 | 0.175 | 0.00 | 0.00 |
| ILE89 | HG12 | 1.00 | 0.088 | 0.00 | 0.00 |
| ILE89 | HG13 | 1.00 | 0.012 | 1.00 | 0.22 |
| ILE89 | HG21 | 1.00 | 0.001 | 1.00 | 0.70 |
| ILE89 | HD11 | 1.00 | 0.004 | 1.00 | 1.15 |
| ILE89 | H | 1.00 | 0.006 | 1.00 | 0.59 |
| TYR90 | H | 1.00 | 0.003 | 1.00 | 0.37 |
| TYR90 | HA | 0.90 | 0.020 | 1.00 | 0.05 |

3.89.3 Detailed Probabilities of ILE89CG1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE89 | 1.00 | 1.00 |
| TYR90 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I89HA | 1.00 |
| I89HB | 1.00 |
| I89HG12 | 1.00 |
| I89HG21 | 1.00 |
| I89HD11 | 1.00 |
| I89H | 1.00 |
| I89HG13 | 1.00 |
| Y90H | 0.96 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE89 | HA | 1.00 | 0.000 | 1.00 | 0.34 |
| ILE89 | HB | 1.00 | 0.002 | 1.00 | 0.19 |
| ILE89 | HG12 | 1.00 | 0.000 | 1.00 | 1.08 |
| ILE89 | HG13 | 1.00 | 0.002 | 1.00 | 1.25 |
| ILE89 | HG21 | 1.00 | 0.003 | 1.00 | 0.38 |
| ILE89 | HD11 | 1.00 | 0.001 | 1.00 | 0.87 |
| ILE89 | H | 1.00 | 0.003 | 1.00 | 0.31 |
| TYR90 | H | 0.96 | 0.005 | 1.00 | 0.05 |

3.89.4 Detailed Probabilities of ILE89CG2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE89 | 1.00 | 1.00 |
| TYR90 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I89HA | 1.00 |
| I89HB | 1.00 |
| I89HG12 | 1.00 |
| I89HG13 | 1.00 |
| I89HG22 | 1.00 |
| I89HD11 | 0.99 |
| I89H | 1.00 |
| Y90H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE89 | HA | 1.00 | 0.001 | 1.00 | 0.73 |
| ILE89 | HB | 1.00 | 0.002 | 1.00 | 0.82 |
| ILE89 | HG12 | 1.00 | 0.008 | 1.00 | 0.45 |
| ILE89 | HG13 | 1.00 | 0.002 | 1.00 | 0.72 |
| ILE89 | HG21 | 1.00 | 0.000 | 1.00 | 18.23 |
| ILE89 | HD11 | 0.99 | 0.001 | 1.00 | 1.70 |
| ILE89 | H | 1.00 | 0.006 | 1.00 | 0.25 |
| TYR90 | H | 0.98 | 0.002 | 1.00 | 0.20 |
| TYR90 | HA | 0.66 | 0.011 | 1.00 | 0.16 |

3.89.5 Detailed Probabilities of ILE89CD1:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE89 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I89HA | 0.97 |
| I89HB | 1.00 |
| I89HG12 | 1.00 |
| I89HG13 | 1.00 |
| I89HG21 | 0.99 |
| I89HD12 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE89 | HA | 0.97 | 0.002 | 1.00 | 0.39 |
| ILE89 | HB | 1.00 | 0.001 | 1.00 | 0.88 |
| ILE89 | HG12 | 1.00 | 0.006 | 1.00 | 1.31 |
| ILE89 | HG13 | 1.00 | 0.004 | 1.00 | 1.75 |
| ILE89 | HG21 | 0.99 | 0.001 | 1.00 | 2.03 |
| ILE89 | HD11 | 1.00 | 0.275 | 0.00 | 0.00 |
| ILE89 | H | 0.94 | 0.007 | 1.00 | 0.48 |

3.89.6 Detailed Probabilities of ILE89N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP88 | 1.00 | 1.00 |
| ILE89 | 1.00 | 1.00 |
| TYR90 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| D88HB3 | 1.00 |
| D88HA | 1.00 |
| D88HB2 | 1.00 |
| D88H | 1.00 |
| I89HA | 1.00 |
| I89HB | 1.00 |
| I89HG12 | 1.00 |
| I89HG13 | 1.00 |
| I89HG21 | 1.00 |
| I89H | 1.00 |
| Y90H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP88 | HA | 1.00 | 0.005 | 1.00 | -327917.00 |
| ASP88 | HB2 | 1.00 | 0.005 | 1.00 | -393719.00 |
| ASP88 | HB3 | 1.00 | 0.005 | 1.00 | -263018.00 |
| ASP88 | H | 1.00 | 0.006 | 1.00 | -1137509.00 |
| ILE89 | HA | 1.00 | 0.000 | 1.00 | -641488.00 |
| ILE89 | HB | 1.00 | 0.001 | 1.00 | -1073309.00 |
| ILE89 | HG12 | 1.00 | 0.004 | 1.00 | -1011016.00 |
| ILE89 | HG13 | 1.00 | 0.007 | 1.00 | -569155.00 |
| ILE89 | HG21 | 1.00 | 0.001 | 1.00 | -412745.00 |
| ILE89 | H | 1.00 | 0.005 | 1.00 | -6725735.00 |
| ILE89 | HD11 | 0.94 | 0.001 | 1.00 | -838871.00 |
| TYR90 | H | 1.00 | 0.000 | 1.00 | -803659.00 |
| TYR90 | HA | 0.95 | 0.003 | 1.00 | -85527.00 |

3.89.7 Detailed Probabilities of ILE89HA:

Overall probability: 0.727

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP88 | 0.50 | 1.00 |
| ILE89 | 1.00 | 1.00 |
| TYR90 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| D88HA | 1.00 |
| I89HB | 1.00 |
| I89HG12 | 1.00 |
| I89HG13 | 1.00 |
| I89HG21 | 1.00 |
| I89HD11 | 0.97 |
| I89H | 1.00 |
| I89HA | 1.00 |
| Y90HA | 1.00 |
| Y90H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP88 | HA | 1.00 | 0.195 | 0.00 | 0.00 |
| ASP88 | H | 0.91 | 0.001 | 1.00 | -113360.00 |
| ILE89 | HA | 1.00 | 0.002 | 1.00 | 5.18 |
| ILE89 | HB | 1.00 | 0.000 | 1.00 | 0.40 |
| ILE89 | HG12 | 1.00 | 0.002 | 1.00 | 0.37 |
| ILE89 | HG13 | 1.00 | 0.000 | 1.00 | 0.34 |
| ILE89 | HG21 | 1.00 | 0.001 | 1.00 | 0.73 |
| ILE89 | HD11 | 0.97 | 0.002 | 1.00 | 0.39 |
| ILE89 | H | 1.00 | 0.000 | 1.00 | -641488.00 |
| TYR90 | HA | 1.00 | 0.053 | 0.00 | 0.00 |
| TYR90 | H | 1.00 | 0.048 | 0.00 | 0.00 |

3.89.8 Detailed Probabilities of ILE89HB:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE89 | 0.71 | 1.00 |
| TYR90 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I89HA | 1.00 |
| I89HG12 | 1.00 |
| I89HG13 | 1.00 |
| I89HG21 | 1.00 |
| I89HD11 | 1.00 |
| I89H | 1.00 |
| I89HB | 1.00 |
| Y90H | 1.00 |

NOESY contacts detailed probability

3.89 ILE(89)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE89 | HA | 1.00 | 0.001 | 1.00 | 0.26 |
| ILE89 | HB | 1.00 | 0.175 | 0.00 | 0.00 |
| ILE89 | HG12 | 1.00 | 0.078 | 0.00 | 0.00 |
| ILE89 | HG13 | 1.00 | 0.002 | 1.00 | 0.19 |
| ILE89 | HG21 | 1.00 | 0.002 | 1.00 | 0.82 |
| ILE89 | HD11 | 1.00 | 0.001 | 1.00 | 0.88 |
| ILE89 | H | 1.00 | 0.001 | 1.00 | -1073309.00 |
| TYR90 | H | 1.00 | 0.005 | 1.00 | -823444.00 |
| TYR90 | HA | 0.90 | 0.010 | 1.00 | 0.10 |

3.89.9 Detailed Probabilities of ILE89HG12:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE89 | 0.71 | 1.00 |
| TYR90 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I89HA | 1.00 |
| I89HB | 1.00 |
| I89HG13 | 1.00 |
| I89HG21 | 1.00 |
| I89HD11 | 1.00 |
| I89H | 1.00 |
| I89HG12 | 1.00 |
| Y90H | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE89 | HA | 1.00 | 0.000 | 1.00 | 0.49 |
| ILE89 | HB | 1.00 | 0.088 | 0.00 | 0.00 |
| ILE89 | HG12 | 1.00 | 0.456 | 0.00 | 0.00 |
| ILE89 | HG13 | 1.00 | 0.000 | 1.00 | 1.08 |
| ILE89 | HG21 | 1.00 | 0.008 | 1.00 | 0.45 |
| ILE89 | HD11 | 1.00 | 0.006 | 1.00 | 1.31 |
| ILE89 | H | 1.00 | 0.004 | 1.00 | -1011016.00 |
| TYR90 | H | 0.99 | 0.006 | 1.00 | -197538.00 |

3.89.10 Detailed Probabilities of ILE89HG13:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE89 | 1.00 | 1.00 |
| TYR90 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I89HA | 1.00 |
| I89HB | 1.00 |
| I89HG12 | 1.00 |
| I89HG21 | 1.00 |
| I89HD11 | 1.00 |
| I89H | 1.00 |
| I89HG13 | 1.00 |
| Y90H | 0.96 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE89 | HA | 1.00 | 0.005 | 1.00 | 0.62 |
| ILE89 | HB | 1.00 | 0.012 | 1.00 | 0.22 |
| ILE89 | HG12 | 1.00 | 0.009 | 1.00 | 1.22 |
| ILE89 | HG13 | 1.00 | 0.002 | 1.00 | 1.25 |
| ILE89 | HG21 | 1.00 | 0.002 | 1.00 | 0.72 |
| ILE89 | HD11 | 1.00 | 0.004 | 1.00 | 1.75 |
| ILE89 | H | 1.00 | 0.007 | 1.00 | -569155.00 |
| TYR90 | H | 0.96 | 0.003 | 1.00 | -164233.00 |

3.89.11 Detailed Probabilities of ILE89HG21:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE89 | 1.00 | 1.00 |
| TYR90 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I89HA | 1.00 |
| I89HB | 1.00 |
| I89HG12 | 1.00 |
| I89HG13 | 1.00 |
| I89HG22 | 1.00 |
| I89HD11 | 0.99 |
| I89H | 1.00 |
| Y90H | 0.98 |

NOESY contacts detailed probability

3.89 ILE(89)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE89 | HA | 1.00 | 0.000 | 1.00 | 0.77 |
| ILE89 | HB | 1.00 | 0.001 | 1.00 | 0.70 |
| ILE89 | HG12 | 1.00 | 0.001 | 1.00 | 0.31 |
| ILE89 | HG13 | 1.00 | 0.003 | 1.00 | 0.38 |
| ILE89 | HG21 | 1.00 | 0.000 | 1.00 | 18.23 |
| ILE89 | HD11 | 0.99 | 0.001 | 1.00 | 2.03 |
| ILE89 | H | 1.00 | 0.001 | 1.00 | -412745.00 |
| TYR90 | H | 0.98 | 0.001 | 1.00 | -410056.00 |
| TYR90 | HA | 0.66 | 0.002 | 1.00 | 0.15 |

3.89.12 Detailed Probabilities of ILE89HD11:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE89 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I89HA | 0.97 |
| I89HB | 1.00 |
| I89HG12 | 1.00 |
| I89HG13 | 1.00 |
| I89HG21 | 0.99 |
| I89HD12 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE89 | HA | 0.97 | 0.002 | 1.00 | 0.47 |
| ILE89 | HB | 1.00 | 0.004 | 1.00 | 1.15 |
| ILE89 | HG12 | 1.00 | 0.002 | 1.00 | 0.93 |
| ILE89 | HG13 | 1.00 | 0.001 | 1.00 | 0.87 |
| ILE89 | HG21 | 0.99 | 0.001 | 1.00 | 1.70 |
| ILE89 | HD11 | 1.00 | 0.275 | 0.00 | 0.00 |
| ILE89 | H | 0.94 | 0.001 | 1.00 | -838871.00 |

3.89.13 Detailed Probabilities of ILE89H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP88 | 1.00 | 1.00 |
| ILE89 | 1.00 | 1.00 |
| TYR90 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| D88HB3 | 1.00 |
| D88HA | 1.00 |
| D88HB2 | 1.00 |
| D88H | 1.00 |
| I89HA | 1.00 |
| I89HB | 1.00 |
| I89HG12 | 1.00 |
| I89HG13 | 1.00 |
| I89HG21 | 1.00 |
| I89H | 1.00 |
| Y90H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP88 | HA | 1.00 | 0.008 | 1.00 | 0.28 |
| ASP88 | HB2 | 1.00 | 0.013 | 1.00 | 0.21 |
| ASP88 | HB3 | 1.00 | 0.007 | 1.00 | 0.19 |
| ASP88 | H | 1.00 | 0.006 | 1.00 | -1636305.00 |
| ILE89 | HA | 1.00 | 0.003 | 1.00 | 0.40 |
| ILE89 | HB | 1.00 | 0.006 | 1.00 | 0.59 |
| ILE89 | HG12 | 1.00 | 0.007 | 1.00 | 0.46 |
| ILE89 | HG13 | 1.00 | 0.003 | 1.00 | 0.31 |
| ILE89 | HG21 | 1.00 | 0.006 | 1.00 | 0.25 |
| ILE89 | H | 1.00 | 0.005 | 1.00 | -6725735.00 |
| ILE89 | HD11 | 0.94 | 0.007 | 1.00 | 0.48 |
| TYR90 | H | 1.00 | 0.002 | 1.00 | -965316.00 |

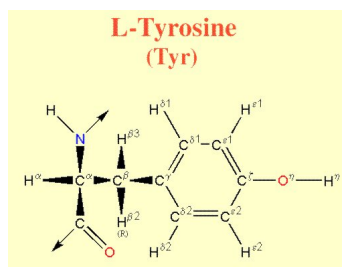


Figure 80: Image from the BMRB

Residue probability: 0.966
 Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 177.681 | 175.405 | 2.122 | 0.000 | 0.000 |
| CA 3.90.1 | 60.106 | 58.279 | 6.333 | 0.833 | 1.000 |
| CB 3.90.2 | 37.732 | 39.527 | 6.280 | 0.960 | 1.000 |
| CD1 3.90.3 | 131.672 | 132.994 | 20.285 | 1.000 | 1.000 |
| CD2 3.90.4 | 131.811 | 133.192 | 23.179 | 1.000 | 1.000 |
| CE1 3.90.5 | 117.857 | 117.867 | 2.496 | 1.000 | 1.000 |
| CE2 3.90.6 | 117.910 | 117.793 | 3.050 | 1.000 | 1.000 |
| N 3.90.7 | 118.599 | 120.136 | 8.494 | 0.923 | 1.000 |
| HA 3.90.8 | 3.977 | 4.610 | 0.592 | 0.777 | 1.000 |
| HB2 3.90.9 | 3.012 | 2.886 | 0.452 | 1.000 | 1.000 |
| HB3 3.90.10 | 3.157 | 2.808 | 0.478 | 1.000 | 1.000 |
| HD1 3.90.11 | 7.007 | 6.912 | 0.327 | 1.000 | 1.000 |
| HD2 3.90.12 | 7.007 | 6.905 | 0.356 | 1.000 | 1.000 |
| HE1 3.90.13 | 6.820 | 6.692 | 0.243 | 1.000 | 1.000 |
| HE2 3.90.14 | 6.820 | 6.690 | 0.252 | 1.000 | 1.000 |
| H 3.90.15 | 9.052 | 8.326 | 0.740 | 1.000 | 1.000 |
| HH | NA | - | - | 0.000 | 0.000 |

3.90.1 Detailed Probabilities of TYR90CA:

Overall probability: 0.833
 Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE89 | 0.67 | 1.00 |
| TYR90 | 1.00 | 1.00 |
| ALA91 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| I89HA | 1.00 |
| Y90HB2 | 1.00 |
| Y90HB3 | 1.00 |
| Y90HD1 | 1.00 |
| Y90HD2 | 1.00 |
| Y90H | 1.00 |
| Y90HA | 1.00 |
| A91H | 1.00 |
| A91HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE89 | HA | 1.00 | 0.053 | 0.00 | 0.00 |
| ILE89 | HB | 0.90 | 0.010 | 1.00 | 0.10 |
| ILE89 | HG21 | 0.68 | 0.002 | 1.00 | 0.15 |
| TYR90 | HA | 1.00 | 0.002 | 1.00 | 4.42 |
| TYR90 | HB2 | 1.00 | 0.001 | 1.00 | 0.41 |
| TYR90 | HB3 | 1.00 | 0.003 | 1.00 | 0.41 |
| TYR90 | HD1 | 1.00 | 0.003 | 1.00 | 0.63 |
| TYR90 | HD2 | 1.00 | 0.003 | 1.00 | 0.63 |
| TYR90 | H | 1.00 | 0.004 | 1.00 | 0.34 |
| TYR90 | HE1 | 0.75 | 0.012 | 1.00 | 0.15 |
| ALA91 | HA | 1.00 | 0.060 | 0.00 | 0.00 |
| ALA91 | H | 1.00 | 0.003 | 1.00 | 0.22 |

3.90.2 Detailed Probabilities of TYR90CB:

Overall probability: 0.960

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TYR90 | 0.95 | 1.00 |
| ALA91 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Y90HA | 1.00 |
| Y90HB3 | 1.00 |
| Y90HD1 | 1.00 |
| Y90HD2 | 1.00 |
| Y90HE2 | 1.00 |
| Y90H | 1.00 |
| Y90HB2 | 1.00 |
| A91H | 1.00 |

NOESY contacts detailed probability

3.90 TYR(90)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TYR90 | HA | 1.00 | 0.034 | 0.60 | 0.00 |
| TYR90 | HB2 | 1.00 | 0.016 | 1.00 | 2.08 |
| TYR90 | HB3 | 1.00 | 0.016 | 1.00 | 2.17 |
| TYR90 | HD1 | 1.00 | 0.002 | 1.00 | 0.25 |
| TYR90 | HD2 | 1.00 | 0.002 | 1.00 | 0.25 |
| TYR90 | HE2 | 1.00 | 0.013 | 1.00 | 0.09 |
| TYR90 | H | 1.00 | 0.003 | 1.00 | 0.29 |
| TYR90 | HE1 | 0.89 | 0.013 | 1.00 | 0.09 |
| ALA91 | H | 1.00 | 0.002 | 1.00 | 0.30 |
| ALA91 | HA | 0.66 | 0.028 | 1.00 | 0.45 |

3.90.3 Detailed Probabilities of TYR90CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TYR90 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Y90HA | 1.00 |
| Y90HB2 | 1.00 |
| Y90HB3 | 1.00 |
| Y90HD2 | 1.00 |
| Y90HE1 | 1.00 |
| Y90HE2 | 1.00 |
| Y90H | 1.00 |
| Y90HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TYR90 | HA | 1.00 | 0.004 | 1.00 | 0.23 |
| TYR90 | HB2 | 1.00 | 0.002 | 1.00 | 0.14 |
| TYR90 | HB3 | 1.00 | 0.000 | 1.00 | 0.18 |
| TYR90 | HD1 | 1.00 | 0.000 | 1.00 | 5.77 |
| TYR90 | HD2 | 1.00 | 0.000 | 1.00 | 5.77 |
| TYR90 | HE1 | 1.00 | 0.006 | 1.00 | 1.84 |
| TYR90 | HE2 | 1.00 | 0.006 | 1.00 | 1.84 |
| TYR90 | H | 1.00 | 0.002 | 1.00 | 0.28 |

3.90.4 Detailed Probabilities of TYR90CD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TYR90 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Y90HA | 1.00 |
| Y90HB2 | 1.00 |
| Y90HB3 | 1.00 |
| Y90HD1 | 1.00 |
| Y90HE1 | 1.00 |
| Y90HE2 | 1.00 |
| Y90H | 0.98 |
| Y90HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TYR90 | HA | 1.00 | 0.004 | 1.00 | 0.23 |
| TYR90 | HB2 | 1.00 | 0.002 | 1.00 | 0.14 |
| TYR90 | HB3 | 1.00 | 0.000 | 1.00 | 0.18 |
| TYR90 | HD1 | 1.00 | 0.000 | 1.00 | 5.77 |
| TYR90 | HD2 | 1.00 | 0.000 | 1.00 | 5.77 |
| TYR90 | HE1 | 1.00 | 0.006 | 1.00 | 1.84 |
| TYR90 | HE2 | 1.00 | 0.006 | 1.00 | 1.84 |
| TYR90 | H | 0.98 | 0.002 | 1.00 | 0.28 |

3.90.5 Detailed Probabilities of TYR90CE1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TYR90 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Y90HD1 | 1.00 |
| Y90HD2 | 1.00 |
| Y90HE2 | 1.00 |
| Y90HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TYR90 | HD1 | 1.00 | 0.002 | 1.00 | 4.32 |
| TYR90 | HD2 | 1.00 | 0.002 | 1.00 | 4.32 |
| TYR90 | HE1 | 1.00 | 0.000 | 1.00 | 13.17 |
| TYR90 | HE2 | 1.00 | 0.000 | 1.00 | 13.17 |
| TYR90 | HA | 0.75 | 0.001 | 1.00 | 0.14 |
| TYR90 | HB2 | 0.89 | 0.004 | 1.00 | 0.10 |
| TYR90 | HB3 | 0.88 | 0.001 | 1.00 | 0.26 |

3.90.6 Detailed Probabilities of TYR90CE2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TYR90 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Y90HB2 | 1.00 |
| Y90HB3 | 1.00 |
| Y90HD1 | 1.00 |
| Y90HD2 | 1.00 |
| Y90HE1 | 1.00 |
| Y90HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TYR90 | HB2 | 1.00 | 0.004 | 1.00 | 0.10 |
| TYR90 | HB3 | 1.00 | 0.001 | 1.00 | 0.26 |
| TYR90 | HD1 | 1.00 | 0.002 | 1.00 | 4.32 |
| TYR90 | HD2 | 1.00 | 0.002 | 1.00 | 4.32 |
| TYR90 | HE1 | 1.00 | 0.000 | 1.00 | 13.17 |
| TYR90 | HE2 | 1.00 | 0.000 | 1.00 | 13.17 |

3.90.7 Detailed Probabilities of TYR90N:

Overall probability: 0.923

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE89 | 0.83 | 1.00 |
| TYR90 | 1.00 | 1.00 |
| ALA91 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I89HA | 1.00 |
| I89HG21 | 0.98 |
| I89H | 1.00 |
| I89HB | 1.00 |
| I89HG12 | 0.99 |
| I89HG13 | 0.96 |
| Y90HA | 1.00 |
| Y90HB2 | 1.00 |
| Y90HB3 | 1.00 |
| Y90HD1 | 1.00 |
| Y90HD2 | 0.98 |
| Y90H | 1.00 |
| A91H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE89 | HA | 1.00 | 0.048 | 0.00 | 0.00 |
| ILE89 | HB | 1.00 | 0.005 | 1.00 | -823444.00 |
| ILE89 | HG12 | 0.99 | 0.006 | 1.00 | -197538.00 |
| ILE89 | HG13 | 0.96 | 0.003 | 1.00 | -164233.00 |
| ILE89 | HG21 | 0.98 | 0.001 | 1.00 | -410056.00 |
| ILE89 | H | 1.00 | 0.002 | 1.00 | -965316.00 |
| TYR90 | HA | 1.00 | 0.000 | 1.00 | -636835.00 |
| TYR90 | HB2 | 1.00 | 0.003 | 1.00 | -682592.00 |
| TYR90 | HB3 | 1.00 | 0.002 | 1.00 | -1039980.00 |
| TYR90 | HD1 | 1.00 | 0.000 | 1.00 | -391579.00 |
| TYR90 | HD2 | 0.98 | 0.000 | 1.00 | -391579.00 |
| TYR90 | H | 1.00 | 0.002 | 1.00 | -7093423.00 |
| ALA91 | H | 1.00 | 0.000 | 1.00 | -922440.00 |

3.90.8 Detailed Probabilities of TYR90HA:

Overall probability: 0.777

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE89 | 1.00 | 1.00 |
| TYR90 | 0.87 | 1.00 |
| ALA91 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| I89HA | 1.00 |
| Y90HB2 | 1.00 |
| Y90HB3 | 1.00 |
| Y90HD1 | 1.00 |
| Y90HD2 | 1.00 |
| Y90H | 1.00 |
| Y90HA | 1.00 |
| A91H | 1.00 |
| A91HA | 1.00 |

NOESY contacts detailed probability

3.90 TYR(90)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE89 | HA | 1.00 | 0.021 | 1.00 | 0.12 |
| ILE89 | HB | 0.90 | 0.020 | 1.00 | 0.05 |
| ILE89 | HG21 | 0.68 | 0.011 | 1.00 | 0.16 |
| ILE89 | H | 0.95 | 0.003 | 1.00 | -85527.00 |
| TYR90 | HA | 1.00 | 0.002 | 1.00 | 4.42 |
| TYR90 | HB2 | 1.00 | 0.034 | 0.60 | 0.00 |
| TYR90 | HB3 | 1.00 | 0.035 | 0.50 | 0.00 |
| TYR90 | HD1 | 1.00 | 0.004 | 1.00 | 0.23 |
| TYR90 | HD2 | 1.00 | 0.004 | 1.00 | 0.23 |
| TYR90 | H | 1.00 | 0.000 | 1.00 | -636835.00 |
| TYR90 | HE1 | 0.75 | 0.001 | 1.00 | 0.14 |
| ALA91 | HA | 1.00 | 0.217 | 0.00 | 0.00 |
| ALA91 | H | 1.00 | 0.041 | 0.00 | 0.00 |

3.90.9 Detailed Probabilities of TYR90HB2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TYR90 | 1.00 | 1.00 |
| ALA91 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Y90HA | 1.00 |
| Y90HB3 | 1.00 |
| Y90HD1 | 1.00 |
| Y90HD2 | 1.00 |
| Y90HE2 | 1.00 |
| Y90H | 1.00 |
| Y90HB2 | 1.00 |
| A91H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TYR90 | HA | 1.00 | 0.001 | 1.00 | 0.41 |
| TYR90 | HB2 | 1.00 | 0.016 | 1.00 | 2.08 |
| TYR90 | HB3 | 1.00 | 0.019 | 1.00 | 2.38 |
| TYR90 | HD1 | 1.00 | 0.002 | 1.00 | 0.14 |
| TYR90 | HD2 | 1.00 | 0.002 | 1.00 | 0.14 |
| TYR90 | HE2 | 1.00 | 0.004 | 1.00 | 0.10 |
| TYR90 | H | 1.00 | 0.003 | 1.00 | -682592.00 |
| TYR90 | HE1 | 0.89 | 0.004 | 1.00 | 0.10 |
| ALA91 | H | 1.00 | 0.003 | 1.00 | -950049.00 |
| ALA91 | HA | 0.66 | 0.010 | 1.00 | 0.07 |

3.90.10 Detailed Probabilities of TYR90HB3:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TYR90 | 1.00 | 1.00 |
| ALA91 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Y90HA | 1.00 |
| Y90HB2 | 1.00 |
| Y90HD1 | 1.00 |
| Y90HD2 | 1.00 |
| Y90HE2 | 1.00 |
| Y90H | 1.00 |
| Y90HB3 | 1.00 |
| A91H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TYR90 | HA | 1.00 | 0.003 | 1.00 | 0.41 |
| TYR90 | HB2 | 1.00 | 0.016 | 1.00 | 2.17 |
| TYR90 | HB3 | 1.00 | 0.005 | 1.00 | 5.26 |
| TYR90 | HD1 | 1.00 | 0.000 | 1.00 | 0.18 |
| TYR90 | HD2 | 1.00 | 0.000 | 1.00 | 0.18 |
| TYR90 | HE2 | 1.00 | 0.001 | 1.00 | 0.26 |
| TYR90 | H | 1.00 | 0.002 | 1.00 | -1039980.00 |
| TYR90 | HE1 | 0.88 | 0.001 | 1.00 | 0.26 |
| ALA91 | H | 1.00 | 0.003 | 1.00 | -1390502.00 |

3.90.11 Detailed Probabilities of TYR90HD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TYR90 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Y90HA | 1.00 |
| Y90HB2 | 1.00 |
| Y90HB3 | 1.00 |
| Y90HD2 | 1.00 |
| Y90HE1 | 1.00 |
| Y90HE2 | 1.00 |
| Y90H | 1.00 |
| Y90HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TYR90 | HA | 1.00 | 0.003 | 1.00 | 0.63 |
| TYR90 | HB2 | 1.00 | 0.002 | 1.00 | 0.25 |
| TYR90 | HB3 | 1.00 | 0.004 | 1.00 | 0.33 |
| TYR90 | HD1 | 1.00 | 0.000 | 1.00 | 5.77 |
| TYR90 | HD2 | 1.00 | 0.000 | 1.00 | 5.77 |
| TYR90 | HE1 | 1.00 | 0.002 | 1.00 | 4.32 |
| TYR90 | HE2 | 1.00 | 0.002 | 1.00 | 4.32 |
| TYR90 | H | 1.00 | 0.000 | 1.00 | -391579.00 |

3.90.12 Detailed Probabilities of TYR90HD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TYR90 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Y90HA | 1.00 |
| Y90HB2 | 1.00 |
| Y90HB3 | 1.00 |
| Y90HD1 | 1.00 |
| Y90HE1 | 1.00 |
| Y90HE2 | 1.00 |
| Y90H | 0.98 |
| Y90HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TYR90 | HA | 1.00 | 0.003 | 1.00 | 0.63 |
| TYR90 | HB2 | 1.00 | 0.002 | 1.00 | 0.25 |
| TYR90 | HB3 | 1.00 | 0.004 | 1.00 | 0.33 |
| TYR90 | HD1 | 1.00 | 0.000 | 1.00 | 5.77 |
| TYR90 | HD2 | 1.00 | 0.000 | 1.00 | 5.77 |
| TYR90 | HE1 | 1.00 | 0.002 | 1.00 | 4.32 |
| TYR90 | HE2 | 1.00 | 0.002 | 1.00 | 4.32 |
| TYR90 | H | 0.98 | 0.000 | 1.00 | -391579.00 |

3.90.13 Detailed Probabilities of TYR90HE1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TYR90 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Y90HD1 | 1.00 |
| Y90HD2 | 1.00 |
| Y90HE2 | 1.00 |
| Y90HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TYR90 | HD1 | 1.00 | 0.006 | 1.00 | 1.84 |
| TYR90 | HD2 | 1.00 | 0.006 | 1.00 | 1.84 |
| TYR90 | HE1 | 1.00 | 0.000 | 1.00 | 13.17 |
| TYR90 | HE2 | 1.00 | 0.000 | 1.00 | 13.17 |
| TYR90 | HA | 0.75 | 0.012 | 1.00 | 0.15 |
| TYR90 | HB2 | 0.89 | 0.013 | 1.00 | 0.09 |
| TYR90 | HB3 | 0.88 | 0.005 | 1.00 | 0.13 |

3.90.14 Detailed Probabilities of TYR90HE2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TYR90 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Y90HB2 | 1.00 |
| Y90HB3 | 1.00 |
| Y90HD1 | 1.00 |
| Y90HD2 | 1.00 |
| Y90HE1 | 1.00 |
| Y90HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TYR90 | HB2 | 1.00 | 0.013 | 1.00 | 0.09 |
| TYR90 | HB3 | 1.00 | 0.005 | 1.00 | 0.13 |
| TYR90 | HD1 | 1.00 | 0.006 | 1.00 | 1.84 |
| TYR90 | HD2 | 1.00 | 0.006 | 1.00 | 1.84 |
| TYR90 | HE1 | 1.00 | 0.000 | 1.00 | 13.17 |
| TYR90 | HE2 | 1.00 | 0.000 | 1.00 | 13.17 |

3.90.15 Detailed Probabilities of TYR90H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE89 | 1.00 | 1.00 |
| TYR90 | 1.00 | 1.00 |
| ALA91 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I89HA | 1.00 |
| I89HG21 | 0.98 |
| I89H | 1.00 |
| I89HB | 1.00 |
| I89HG12 | 0.99 |
| I89HG13 | 0.96 |
| Y90HA | 1.00 |
| Y90HB2 | 1.00 |
| Y90HB3 | 1.00 |
| Y90HD1 | 1.00 |
| Y90HD2 | 0.98 |
| Y90H | 1.00 |
| A91H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE89 | HA | 1.00 | 0.003 | 1.00 | 0.11 |
| ILE89 | HB | 1.00 | 0.003 | 1.00 | 0.37 |
| ILE89 | HG12 | 0.99 | 0.003 | 1.00 | 0.08 |
| ILE89 | HG13 | 0.96 | 0.005 | 1.00 | 0.05 |
| ILE89 | HG21 | 0.98 | 0.002 | 1.00 | 0.20 |
| ILE89 | H | 1.00 | 0.000 | 1.00 | -803659.00 |
| TYR90 | HA | 1.00 | 0.004 | 1.00 | 0.34 |
| TYR90 | HB2 | 1.00 | 0.003 | 1.00 | 0.29 |
| TYR90 | HB3 | 1.00 | 0.003 | 1.00 | 0.33 |
| TYR90 | HD1 | 1.00 | 0.002 | 1.00 | 0.28 |
| TYR90 | HD2 | 0.98 | 0.002 | 1.00 | 0.28 |
| TYR90 | H | 1.00 | 0.002 | 1.00 | -7093423.00 |
| ALA91 | H | 1.00 | 0.001 | 1.00 | -1131871.00 |

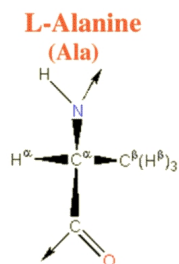
3.91 ALA(91)

Figure 81: Image from the BMRB

Residue probability: 0.829

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-----------|-------------|---------|--------|---------------------|--------------------|
| CA 3.91.1 | 55.144 | 53.289 | 3.425 | 0.572 | 1.000 |
| CB 3.91.2 | 18.066 | 19.355 | 4.103 | 1.000 | 1.000 |
| N 3.91.3 | 119.071 | 123.100 | 4.487 | 0.900 | 1.000 |
| HA 3.91.4 | 4.039 | 4.254 | 0.459 | 0.500 | 1.000 |
| HB 3.91.5 | 1.561 | 1.346 | 0.258 | 1.000 | 1.000 |
| H 3.91.6 | 7.947 | 8.206 | 0.601 | 1.000 | 1.000 |

3.91.1 Detailed Probabilities of ALA91CA:

Overall probability: 0.572

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TYR90 | 0.50 | 1.00 |
| ALA91 | 0.67 | 1.00 |
| THR92 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Y90HA | 1.00 |
| A91H | 1.00 |
| A91HB1 | 1.00 |
| A91HA | 1.00 |
| T92H | 1.00 |
| T92HA | 1.00 |

NOESY contacts detailed probability

3.91 ALA(91)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TYR90 | HA | 1.00 | 0.217 | 0.00 | 0.00 |
| TYR90 | HB2 | 0.66 | 0.010 | 1.00 | 0.07 |
| ALA91 | HA | 1.00 | 0.155 | 0.00 | 0.00 |
| ALA91 | HB1 | 1.00 | 0.012 | 1.00 | 2.57 |
| ALA91 | H | 1.00 | 0.000 | 1.00 | 0.87 |
| THR92 | HA | 1.00 | 0.217 | 0.00 | 0.00 |
| THR92 | H | 1.00 | 0.010 | 1.00 | 0.87 |

3.91.2 Detailed Probabilities of ALA91CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA91 | 1.00 | 1.00 |
| THR92 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A91HA | 1.00 |
| A91H | 1.00 |
| A91HB2 | 1.00 |
| T92H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA91 | HA | 1.00 | 0.002 | 1.00 | 2.44 |
| ALA91 | HB1 | 1.00 | 0.010 | 1.00 | 50.79 |
| ALA91 | H | 1.00 | 0.000 | 1.00 | 2.98 |
| THR92 | H | 1.00 | 0.010 | 1.00 | 2.98 |

3.91.3 Detailed Probabilities of ALA91N:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TYR90 | 0.83 | 1.00 |
| ALA91 | 1.00 | 1.00 |
| THR92 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Y90HB3 | 1.00 |
| Y90HA | 1.00 |
| Y90H | 1.00 |
| Y90HB2 | 1.00 |
| A91HA | 1.00 |
| A91HB1 | 1.00 |
| A91H | 1.00 |
| T92H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TYR90 | HA | 1.00 | 0.041 | 0.00 | 0.00 |
| TYR90 | HB2 | 1.00 | 0.003 | 1.00 | -950049.00 |
| TYR90 | HB3 | 1.00 | 0.003 | 1.00 | -1390502.00 |
| TYR90 | H | 1.00 | 0.001 | 1.00 | -1131871.00 |
| TYR90 | HD1 | 0.79 | 0.001 | 1.00 | -538464.00 |
| TYR90 | HD2 | 0.68 | 0.001 | 1.00 | -538464.00 |
| ALA91 | HA | 1.00 | 0.009 | 1.00 | -1357798.00 |
| ALA91 | HB1 | 1.00 | 0.012 | 1.00 | -5116620.00 |
| ALA91 | H | 1.00 | 0.002 | 1.00 | -21352072.00 |
| THR92 | H | 1.00 | 0.012 | 1.00 | -21352072.00 |

3.91.4 Detailed Probabilities of ALA91HA:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TYR90 | 0.67 | 1.00 |
| ALA91 | 0.67 | 1.00 |
| THR92 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Y90HA | 1.00 |
| A91H | 1.00 |
| A91HB1 | 1.00 |
| A91HA | 1.00 |
| T92H | 1.00 |
| T92HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TYR90 | HA | 1.00 | 0.060 | 0.00 | 0.00 |
| TYR90 | HB2 | 0.66 | 0.028 | 1.00 | 0.45 |
| TYR90 | HB3 | 0.85 | 0.027 | 1.00 | 0.62 |
| ALA91 | HA | 1.00 | 0.155 | 0.00 | 0.00 |
| ALA91 | HB1 | 1.00 | 0.002 | 1.00 | 2.44 |
| ALA91 | H | 1.00 | 0.009 | 1.00 | -1357798.00 |
| THR92 | HA | 1.00 | 0.154 | 0.00 | 0.00 |
| THR92 | H | 1.00 | 0.060 | 0.00 | 0.00 |

3.91.5 Detailed Probabilities of ALA91HB1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA91 | 1.00 | 1.00 |
| THR92 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A91HA | 1.00 |
| A91H | 1.00 |
| A91HB2 | 1.00 |
| T92H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA91 | HA | 1.00 | 0.012 | 1.00 | 2.57 |
| ALA91 | HB1 | 1.00 | 0.010 | 1.00 | 50.79 |
| ALA91 | H | 1.00 | 0.012 | 1.00 | -5116620.00 |
| THR92 | H | 1.00 | 0.013 | 1.00 | -1806972.00 |
| THR92 | HA | 0.71 | 0.010 | 1.00 | 0.19 |

3.91.6 Detailed Probabilities of ALA91H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| TYR90 | 1.00 | 1.00 |
| ALA91 | 1.00 | 1.00 |
| THR92 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| Y90HB3 | 1.00 |
| Y90HA | 1.00 |
| Y90H | 1.00 |
| Y90HB2 | 1.00 |
| A91HA | 1.00 |
| A91HB1 | 1.00 |
| A91H | 1.00 |
| T92H | 1.00 |

NOESY contacts detailed probability

3.91 ALA(91)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| TYR90 | HA | 1.00 | 0.003 | 1.00 | 0.22 |
| TYR90 | HB2 | 1.00 | 0.002 | 1.00 | 0.30 |
| TYR90 | HB3 | 1.00 | 0.001 | 1.00 | 0.39 |
| TYR90 | H | 1.00 | 0.000 | 1.00 | -922440.00 |
| TYR90 | HD1 | 0.79 | 0.004 | 1.00 | 0.08 |
| TYR90 | HD2 | 0.68 | 0.004 | 1.00 | 0.08 |
| ALA91 | HA | 1.00 | 0.000 | 1.00 | 0.87 |
| ALA91 | HB1 | 1.00 | 0.000 | 1.00 | 2.98 |
| ALA91 | H | 1.00 | 0.002 | 1.00 | -21352072.00 |
| THR92 | H | 1.00 | 0.003 | 1.00 | -11257836.00 |

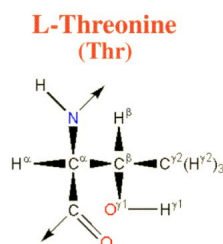
3.92 THR(92)

Figure 82: Image from the BMRB

Residue probability: 0.780

Residue probability confidence: 0.858

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 176.823 | 174.627 | 1.788 | 0.000 | 0.000 |
| CA 3.92.1 | 66.793 | 62.330 | 4.136 | 0.500 | 0.875 |
| CB 3.92.2 | 68.301 | 69.395 | 4.500 | 1.000 | 0.833 |
| CG2 3.92.3 | 21.783 | 21.588 | 1.595 | 0.503 | 0.833 |
| N 3.92.4 | 114.461 | 115.370 | 5.913 | 0.875 | 0.889 |
| HA 3.92.5 | 3.977 | 4.461 | 0.626 | 0.778 | 0.875 |
| HB 3.92.6 | 4.200 | 4.172 | 0.855 | 1.000 | 0.833 |
| HG2 3.92.7 | 1.043 | 1.134 | 0.349 | 0.833 | 0.833 |
| H 3.92.8 | 7.937 | 8.272 | 1.597 | 0.750 | 0.889 |
| HG1 | NA | – | – | 0.000 | 0.000 |

3.92.1 Detailed Probabilities of THR92CA:

Overall probability: 0.500

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA91 | 0.50 | 1.00 |
| THR92 | 0.50 | 0.80 |
| ILE93 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| A91HA | 1.00 |
| T92HB | 1.00 |
| T92HG21 | 1.00 |
| T92H | 1.00 |
| T92HG1 | 1.00 |
| T92HA | 1.00 |
| I93HA | 1.00 |
| I93H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA91 | HA | 1.00 | 0.154 | 0.00 | 0.00 |
| ALA91 | HB1 | 0.67 | 0.010 | 1.00 | 0.19 |
| THR92 | HA | 1.00 | 0.216 | 0.00 | 0.00 |
| THR92 | HB | 1.00 | 0.007 | 1.00 | 0.63 |
| THR92 | HG21 | 1.00 | 0.004 | 1.00 | 1.36 |
| THR92 | H | 1.00 | 0.309 | 0.00 | 0.00 |
| ILE93 | HA | 1.00 | 0.316 | 0.00 | 0.00 |
| ILE93 | H | 1.00 | 0.007 | 1.00 | 0.26 |

3.92.2 Detailed Probabilities of THR92CB:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR92 | 1.00 | 0.80 |
| ILE93 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T92HA | 1.00 |
| T92HG21 | 1.00 |
| T92H | 1.00 |
| T92HG1 | 1.00 |
| T92HB | 1.00 |
| I93H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR92 | HA | 1.00 | 0.003 | 1.00 | 0.38 |
| THR92 | HB | 1.00 | 0.002 | 1.00 | 3.09 |
| THR92 | HG21 | 1.00 | 0.004 | 1.00 | 1.11 |
| THR92 | H | 1.00 | 0.009 | 1.00 | 0.83 |
| ILE93 | H | 1.00 | 0.000 | 1.00 | 0.42 |
| ILE93 | HA | 0.90 | 0.012 | 1.00 | 0.07 |

3.92.3 Detailed Probabilities of THR92CG2:

Overall probability: 0.503

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR92 | 0.50 | 0.80 |
| ILE93 | 0.51 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T92HA | 1.00 |
| T92HB | 1.00 |
| T92HG22 | 1.00 |
| T92H | 1.00 |
| T92HG1 | 1.00 |
| I93H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR92 | HA | 1.00 | 0.006 | 1.00 | 1.76 |
| THR92 | HB | 1.00 | 0.001 | 1.00 | 1.44 |
| THR92 | HG21 | 1.00 | 0.198 | 0.00 | 0.00 |
| THR92 | H | 1.00 | 0.460 | 0.00 | 0.00 |
| ILE93 | H | 0.98 | 0.161 | 0.02 | 0.00 |
| ILE93 | HA | 0.50 | 0.002 | 1.00 | 0.12 |

3.92.4 Detailed Probabilities of THR92N:

Overall probability: 0.875

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA91 | 0.67 | 1.00 |
| THR92 | 1.00 | 0.80 |
| ILE93 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| A91HB1 | 1.00 |
| A91H | 1.00 |
| A91HA | 1.00 |
| T92HA | 1.00 |
| T92HB | 1.00 |
| T92HG21 | 1.00 |
| T92HG1 | 1.00 |
| T92H | 1.00 |
| I93H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA91 | HA | 1.00 | 0.060 | 0.00 | 0.00 |
| ALA91 | HB1 | 1.00 | 0.013 | 1.00 | -1806972.00 |
| ALA91 | H | 1.00 | 0.003 | 1.00 | -11257836.00 |
| THR92 | HA | 1.00 | 0.002 | 1.00 | -1251608.00 |
| THR92 | HB | 1.00 | 0.004 | 1.00 | -1698182.00 |
| THR92 | HG21 | 1.00 | 0.006 | 1.00 | -596857.00 |
| THR92 | H | 1.00 | 0.007 | 1.00 | -11257836.00 |
| ILE93 | H | 1.00 | 0.000 | 1.00 | -993148.00 |

3.92.5 Detailed Probabilities of THR92HA:

Overall probability: 0.778

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA91 | 0.00 | 1.00 |
| THR92 | 0.75 | 0.80 |
| ILE93 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| A91HA | 1.00 |
| T92HB | 1.00 |
| T92HG21 | 1.00 |
| T92H | 1.00 |
| T92HG1 | 1.00 |
| T92HA | 1.00 |
| I93HA | 1.00 |
| I93H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA91 | HA | 1.00 | 0.217 | 0.00 | 0.00 |
| THR92 | HA | 1.00 | 0.216 | 0.00 | 0.00 |
| THR92 | HB | 1.00 | 0.003 | 1.00 | 0.38 |
| THR92 | HG21 | 1.00 | 0.006 | 1.00 | 1.76 |
| THR92 | H | 1.00 | 0.002 | 1.00 | -1251608.00 |
| ILE93 | HA | 1.00 | 0.007 | 1.00 | 0.06 |
| ILE93 | H | 1.00 | 0.002 | 1.00 | -563391.00 |
| ILE93 | HB | 0.59 | 0.000 | 1.00 | 0.22 |
| ILE93 | HG12 | 0.57 | 0.000 | 1.00 | 0.05 |

3.92.6 Detailed Probabilities of THR92HB:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR92 | 1.00 | 0.80 |
| ILE93 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T92HA | 1.00 |
| T92HG21 | 1.00 |
| T92H | 1.00 |
| T92HG1 | 1.00 |
| T92HB | 1.00 |
| I93H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR92 | HA | 1.00 | 0.007 | 1.00 | 0.63 |
| THR92 | HB | 1.00 | 0.002 | 1.00 | 3.09 |
| THR92 | HG21 | 1.00 | 0.001 | 1.00 | 1.44 |
| THR92 | H | 1.00 | 0.004 | 1.00 | -1698182.00 |
| ILE93 | H | 1.00 | 0.003 | 1.00 | -836618.00 |
| ILE93 | HA | 0.90 | 0.002 | 1.00 | 0.06 |

3.92.7 Detailed Probabilities of THR92HG21:

Overall probability: 0.833

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR92 | 0.75 | 0.80 |
| ILE93 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T92HA | 1.00 |
| T92HB | 1.00 |
| T92HG22 | 1.00 |
| T92H | 1.00 |
| T92HG1 | 1.00 |
| I93H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR92 | HA | 1.00 | 0.004 | 1.00 | 1.36 |
| THR92 | HB | 1.00 | 0.004 | 1.00 | 1.11 |
| THR92 | HG21 | 1.00 | 0.198 | 0.00 | 0.00 |
| THR92 | H | 1.00 | 0.006 | 1.00 | -596857.00 |
| ILE93 | H | 0.98 | 0.001 | 1.00 | -423365.00 |
| ILE93 | HA | 0.50 | 0.004 | 1.00 | 0.20 |

3.92.8 Detailed Probabilities of THR92H:

Overall probability: 0.750

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA91 | 1.00 | 1.00 |
| THR92 | 0.50 | 0.80 |
| ILE93 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| A91HB1 | 1.00 |
| A91H | 1.00 |
| A91HA | 1.00 |
| T92HA | 1.00 |
| T92HB | 1.00 |
| T92HG21 | 1.00 |
| T92HG1 | 1.00 |
| T92H | 1.00 |
| I93H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA91 | HA | 1.00 | 0.010 | 1.00 | 0.87 |
| ALA91 | HB1 | 1.00 | 0.010 | 1.00 | 2.98 |
| ALA91 | H | 1.00 | 0.012 | 1.00 | -21352072.00 |
| THR92 | HA | 1.00 | 0.309 | 0.00 | 0.00 |
| THR92 | HB | 1.00 | 0.009 | 1.00 | 0.83 |
| THR92 | HG21 | 1.00 | 0.460 | 0.00 | 0.00 |
| THR92 | H | 1.00 | 0.007 | 1.00 | -11257836.00 |
| ILE93 | H | 1.00 | 0.008 | 1.00 | -1005309.00 |

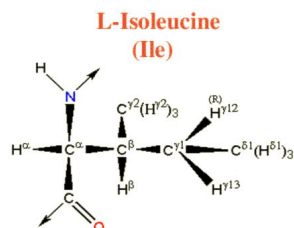
3.93 ILE(93)

Figure 83: Image from the BMRB

Residue probability: 0.807

Residue probability confidence: 0.987

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|--------------|-------------|---------|--------|---------------------|--------------------|
| C | 177.135 | 175.926 | 2.710 | 0.000 | 0.000 |
| CA 3.93.1 | 66.413 | 61.717 | 4.152 | 0.752 | 1.000 |
| CB 3.93.2 | 37.978 | 38.702 | 3.945 | 0.889 | 1.000 |
| CG1 3.93.3 | 29.576 | 27.785 | 2.037 | 0.714 | 1.000 |
| CG2 3.93.4 | 17.769 | 17.574 | 1.928 | 0.667 | 1.000 |
| CD1 3.93.5 | 14.039 | 13.545 | 3.646 | 1.000 | 1.000 |
| N 3.93.6 | 121.493 | 121.467 | 6.098 | 1.000 | 0.917 |
| HA 3.93.7 | 3.523 | 4.185 | 1.403 | 0.833 | 1.000 |
| HB 3.93.8 | 1.852 | 1.776 | 0.310 | 0.750 | 1.000 |
| HG12 3.93.9 | 0.626 | 1.271 | 0.411 | 0.750 | 1.000 |
| HG13 3.93.10 | 1.947 | 1.186 | 0.426 | 0.571 | 1.000 |
| HG2 3.93.11 | 0.884 | 0.762 | 0.283 | 0.778 | 1.000 |
| HD1 3.93.12 | 0.507 | 0.668 | 0.293 | 0.861 | 1.000 |
| H 3.93.13 | 8.253 | 8.301 | 0.685 | 0.924 | 0.917 |

3.93.1 Detailed Probabilities of ILE93CA:

Overall probability: 0.752

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR92 | 1.00 | 1.00 |
| ILE93 | 0.72 | 1.00 |
| MET94 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T92HA | 1.00 |
| I93HB | 1.00 |
| I93HG12 | 1.00 |
| I93HG13 | 1.00 |
| I93HG21 | 1.00 |
| I93HD11 | 0.97 |
| I93H | 1.00 |
| I93HA | 1.00 |
| M94HA | 1.00 |
| M94H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR92 | HA | 1.00 | 0.007 | 1.00 | 0.06 |
| THR92 | HB | 0.90 | 0.002 | 1.00 | 0.06 |
| THR92 | HG21 | 0.52 | 0.004 | 1.00 | 0.20 |
| ILE93 | HA | 1.00 | 0.003 | 1.00 | 4.88 |
| ILE93 | HB | 1.00 | 0.005 | 1.00 | 0.31 |
| ILE93 | HG12 | 1.00 | 0.071 | 0.00 | 0.00 |
| ILE93 | HG13 | 1.00 | 0.003 | 1.00 | 0.46 |
| ILE93 | HG21 | 1.00 | 0.002 | 1.00 | 0.89 |
| ILE93 | HD11 | 0.97 | 0.048 | 0.03 | 0.00 |
| ILE93 | H | 1.00 | 0.003 | 1.00 | 0.58 |
| MET94 | HA | 1.00 | 0.077 | 0.00 | 0.00 |
| MET94 | H | 1.00 | 0.005 | 1.00 | 0.22 |

3.93.2 Detailed Probabilities of ILE93CB:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE93 | 0.86 | 1.00 |
| MET94 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I93HA | 1.00 |
| I93HG12 | 1.00 |
| I93HG13 | 1.00 |
| I93HG21 | 1.00 |
| I93HD11 | 1.00 |
| I93H | 1.00 |
| I93HB | 1.00 |
| M94H | 1.00 |

NOESY contacts detailed probability

3.93 ILE(93)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE93 | HA | 1.00 | 0.002 | 1.00 | 0.19 |
| ILE93 | HB | 1.00 | 0.001 | 1.00 | 2.02 |
| ILE93 | HG12 | 1.00 | 0.003 | 1.00 | 0.25 |
| ILE93 | HG13 | 1.00 | 0.094 | 0.00 | 0.00 |
| ILE93 | HG21 | 1.00 | 0.005 | 1.00 | 0.81 |
| ILE93 | HD11 | 1.00 | 0.003 | 1.00 | 0.61 |
| ILE93 | H | 1.00 | 0.000 | 1.00 | 0.54 |
| MET94 | H | 1.00 | 0.007 | 1.00 | 0.30 |
| MET94 | HA | 0.89 | 0.002 | 1.00 | 0.05 |

3.93.3 Detailed Probabilities of ILE93CG1:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE93 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I93HA | 1.00 |
| I93HB | 1.00 |
| I93HG12 | 1.00 |
| I93HG21 | 1.00 |
| I93HD11 | 1.00 |
| I93H | 1.00 |
| I93HG13 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE93 | HA | 1.00 | 0.001 | 1.00 | 0.25 |
| ILE93 | HB | 1.00 | 0.049 | 0.00 | 0.00 |
| ILE93 | HG12 | 1.00 | 0.004 | 1.00 | 0.86 |
| ILE93 | HG13 | 1.00 | 0.144 | 0.00 | 0.00 |
| ILE93 | HG21 | 1.00 | 0.007 | 1.00 | 0.41 |
| ILE93 | HD11 | 1.00 | 0.000 | 1.00 | 0.80 |
| ILE93 | H | 1.00 | 0.005 | 1.00 | 0.32 |

3.93.4 Detailed Probabilities of ILE93CG2:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE93 | 0.57 | 1.00 |
| MET94 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I93HA | 1.00 |
| I93HB | 1.00 |
| I93HG12 | 1.00 |
| I93HG13 | 1.00 |
| I93HG22 | 1.00 |
| I93HD11 | 0.99 |
| I93H | 1.00 |
| M94H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE93 | HA | 1.00 | 0.003 | 1.00 | 0.89 |
| ILE93 | HB | 1.00 | 0.015 | 1.00 | 1.47 |
| ILE93 | HG12 | 1.00 | 0.121 | 0.00 | 0.00 |
| ILE93 | HG13 | 1.00 | 0.110 | 0.00 | 0.00 |
| ILE93 | HG21 | 1.00 | 0.137 | 0.00 | 0.00 |
| ILE93 | HD11 | 0.99 | 0.002 | 1.00 | 2.76 |
| ILE93 | H | 1.00 | 0.000 | 1.00 | 0.41 |
| MET94 | H | 0.99 | 0.001 | 1.00 | 0.38 |
| MET94 | HA | 0.70 | 0.001 | 1.00 | 0.15 |

3.93.5 Detailed Probabilities of ILE93CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE93 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I93HA | 0.97 |
| I93HB | 1.00 |
| I93HG12 | 1.00 |
| I93HG13 | 1.00 |
| I93HG21 | 0.99 |
| I93HD12 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE93 | HA | 0.97 | 0.000 | 1.00 | 0.36 |
| ILE93 | HB | 1.00 | 0.008 | 1.00 | 0.98 |
| ILE93 | HG12 | 1.00 | 0.002 | 1.00 | 2.12 |
| ILE93 | HG13 | 1.00 | 0.000 | 1.00 | 1.42 |
| ILE93 | HG21 | 0.99 | 0.001 | 1.00 | 2.45 |
| ILE93 | HD11 | 1.00 | 0.005 | 1.00 | 30.00 |
| ILE93 | H | 0.94 | 0.000 | 1.00 | 0.44 |

3.93.6 Detailed Probabilities of ILE93N:

Overall probability: 1.000

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR92 | 1.00 | 0.80 |
| ILE93 | 1.00 | 1.00 |
| MET94 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T92H | 1.00 |
| T92HB | 1.00 |
| T92HG23 | 0.98 |
| T92HG1 | 0.97 |
| T92HA | 1.00 |
| I93HA | 1.00 |
| I93HB | 1.00 |
| I93HG12 | 1.00 |
| I93HG13 | 1.00 |
| I93HG21 | 1.00 |
| I93H | 1.00 |
| M94H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR92 | HA | 1.00 | 0.002 | 1.00 | -563391.00 |
| THR92 | HB | 1.00 | 0.003 | 1.00 | -836618.00 |
| THR92 | HG21 | 0.98 | 0.001 | 1.00 | -423365.00 |
| THR92 | H | 1.00 | 0.008 | 1.00 | -1005309.00 |
| ILE93 | HA | 1.00 | 0.001 | 1.00 | -677107.00 |
| ILE93 | HB | 1.00 | 0.000 | 1.00 | -1541024.00 |
| ILE93 | HG12 | 1.00 | 0.003 | 1.00 | -763307.00 |
| ILE93 | HG13 | 1.00 | 0.000 | 1.00 | -1230102.00 |
| ILE93 | HG21 | 1.00 | 0.004 | 1.00 | -609125.00 |
| ILE93 | H | 1.00 | 0.000 | 1.00 | -7216570.00 |
| ILE93 | HD11 | 0.94 | 0.002 | 1.00 | -811379.00 |
| MET94 | H | 1.00 | 0.006 | 1.00 | -923181.00 |
| MET94 | HB2 | 0.50 | 0.008 | 1.00 | -110771.00 |

3.93.7 Detailed Probabilities of ILE93HA:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR92 | 0.67 | 1.00 |
| ILE93 | 1.00 | 1.00 |
| MET94 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T92HA | 1.00 |
| I93HB | 1.00 |
| I93HG12 | 1.00 |
| I93HG13 | 1.00 |
| I93HG21 | 1.00 |
| I93HD11 | 0.97 |
| I93H | 1.00 |
| I93HA | 1.00 |
| M94HA | 1.00 |
| M94H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR92 | HA | 1.00 | 0.316 | 0.00 | 0.00 |
| THR92 | HB | 0.90 | 0.012 | 1.00 | 0.07 |
| THR92 | HG21 | 0.52 | 0.002 | 1.00 | 0.12 |
| ILE93 | HA | 1.00 | 0.003 | 1.00 | 4.88 |
| ILE93 | HB | 1.00 | 0.002 | 1.00 | 0.19 |
| ILE93 | HG12 | 1.00 | 0.005 | 1.00 | 0.21 |
| ILE93 | HG13 | 1.00 | 0.001 | 1.00 | 0.25 |
| ILE93 | HG21 | 1.00 | 0.003 | 1.00 | 0.89 |
| ILE93 | HD11 | 0.97 | 0.000 | 1.00 | 0.36 |
| ILE93 | H | 1.00 | 0.001 | 1.00 | -677107.00 |
| MET94 | HA | 1.00 | 0.258 | 0.00 | 0.00 |
| MET94 | H | 1.00 | 0.006 | 1.00 | -238315.00 |

3.93.8 Detailed Probabilities of ILE93HB:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE93 | 0.71 | 1.00 |
| MET94 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I93HA | 1.00 |
| I93HG12 | 1.00 |
| I93HG13 | 1.00 |
| I93HG21 | 1.00 |
| I93HD11 | 1.00 |
| I93H | 1.00 |
| I93HB | 1.00 |
| M94H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE93 | HA | 1.00 | 0.005 | 1.00 | 0.31 |
| ILE93 | HB | 1.00 | 0.001 | 1.00 | 2.02 |
| ILE93 | HG12 | 1.00 | 0.095 | 0.00 | 0.00 |
| ILE93 | HG13 | 1.00 | 0.049 | 0.00 | 0.00 |
| ILE93 | HG21 | 1.00 | 0.015 | 1.00 | 1.47 |
| ILE93 | HD11 | 1.00 | 0.008 | 1.00 | 0.98 |
| ILE93 | H | 1.00 | 0.000 | 1.00 | -1541024.00 |
| MET94 | H | 1.00 | 0.000 | 1.00 | -1062626.00 |

3.93.9 Detailed Probabilities of ILE93HG12:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE93 | 0.71 | 1.00 |
| MET94 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I93HA | 1.00 |
| I93HB | 1.00 |
| I93HG13 | 1.00 |
| I93HG21 | 1.00 |
| I93HD11 | 1.00 |
| I93H | 1.00 |
| I93HG12 | 1.00 |
| M94H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE93 | HA | 1.00 | 0.071 | 0.00 | 0.00 |
| ILE93 | HB | 1.00 | 0.003 | 1.00 | 0.25 |
| ILE93 | HG12 | 1.00 | 0.010 | 1.00 | 0.67 |
| ILE93 | HG13 | 1.00 | 0.004 | 1.00 | 0.86 |
| ILE93 | HG21 | 1.00 | 0.121 | 0.00 | 0.00 |
| ILE93 | HD11 | 1.00 | 0.002 | 1.00 | 2.12 |
| ILE93 | H | 1.00 | 0.003 | 1.00 | -763307.00 |
| MET94 | H | 0.97 | 0.004 | 1.00 | -120159.00 |

3.93.10 Detailed Probabilities of ILE93HG13:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE93 | 0.57 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I93HA | 1.00 |
| I93HB | 1.00 |
| I93HG12 | 1.00 |
| I93HG21 | 1.00 |
| I93HD11 | 1.00 |
| I93H | 1.00 |
| I93HG13 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE93 | HA | 1.00 | 0.003 | 1.00 | 0.46 |
| ILE93 | HB | 1.00 | 0.094 | 0.00 | 0.00 |
| ILE93 | HG12 | 1.00 | 0.000 | 1.00 | 0.69 |
| ILE93 | HG13 | 1.00 | 0.144 | 0.00 | 0.00 |
| ILE93 | HG21 | 1.00 | 0.110 | 0.00 | 0.00 |
| ILE93 | HD11 | 1.00 | 0.000 | 1.00 | 1.42 |
| ILE93 | H | 1.00 | 0.000 | 1.00 | -1230102.00 |

3.93.11 Detailed Probabilities of ILE93HG21:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE93 | 0.71 | 1.00 |
| MET94 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I93HA | 1.00 |
| I93HB | 1.00 |
| I93HG12 | 1.00 |
| I93HG13 | 1.00 |
| I93HG22 | 1.00 |
| I93HD11 | 0.99 |
| I93H | 1.00 |
| M94H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE93 | HA | 1.00 | 0.002 | 1.00 | 0.89 |
| ILE93 | HB | 1.00 | 0.005 | 1.00 | 0.81 |
| ILE93 | HG12 | 1.00 | 0.248 | 0.00 | 0.00 |
| ILE93 | HG13 | 1.00 | 0.007 | 1.00 | 0.41 |
| ILE93 | HG21 | 1.00 | 0.137 | 0.00 | 0.00 |
| ILE93 | HD11 | 0.99 | 0.001 | 1.00 | 2.45 |
| ILE93 | H | 1.00 | 0.004 | 1.00 | -609125.00 |
| MET94 | H | 0.99 | 0.008 | 1.00 | -555329.00 |
| MET94 | HA | 0.70 | 0.010 | 1.00 | 0.25 |

3.93.12 Detailed Probabilities of ILE93HD11:

Overall probability: 0.861

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE93 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I93HA | 0.97 |
| I93HB | 1.00 |
| I93HG12 | 1.00 |
| I93HG13 | 1.00 |
| I93HG21 | 0.99 |
| I93HD12 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE93 | HA | 0.97 | 0.048 | 0.03 | 0.00 |
| ILE93 | HB | 1.00 | 0.003 | 1.00 | 0.61 |
| ILE93 | HG12 | 1.00 | 0.001 | 1.00 | 0.60 |
| ILE93 | HG13 | 1.00 | 0.000 | 1.00 | 0.80 |
| ILE93 | HG21 | 0.99 | 0.002 | 1.00 | 2.76 |
| ILE93 | HD11 | 1.00 | 0.005 | 1.00 | 30.00 |
| ILE93 | H | 0.94 | 0.002 | 1.00 | -811379.00 |

3.93.13 Detailed Probabilities of ILE93H:

Overall probability: 0.924

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR92 | 0.75 | 0.80 |
| ILE93 | 1.00 | 1.00 |
| MET94 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T92H | 1.00 |
| T92HB | 1.00 |
| T92HG23 | 0.98 |
| T92HG1 | 0.97 |
| T92HA | 1.00 |
| I93HA | 1.00 |
| I93HB | 1.00 |
| I93HG12 | 1.00 |
| I93HG13 | 1.00 |
| I93HG21 | 1.00 |
| I93H | 1.00 |
| M94H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR92 | HA | 1.00 | 0.007 | 1.00 | 0.26 |
| THR92 | HB | 1.00 | 0.000 | 1.00 | 0.42 |
| THR92 | HG21 | 0.98 | 0.161 | 0.02 | 0.00 |
| THR92 | H | 1.00 | 0.000 | 1.00 | -993148.00 |
| ILE93 | HA | 1.00 | 0.003 | 1.00 | 0.58 |
| ILE93 | HB | 1.00 | 0.000 | 1.00 | 0.54 |
| ILE93 | HG12 | 1.00 | 0.003 | 1.00 | 0.17 |
| ILE93 | HG13 | 1.00 | 0.005 | 1.00 | 0.32 |
| ILE93 | HG21 | 1.00 | 0.000 | 1.00 | 0.41 |
| ILE93 | H | 1.00 | 0.000 | 1.00 | -7216570.00 |
| ILE93 | HD11 | 0.94 | 0.000 | 1.00 | 0.44 |
| MET94 | H | 1.00 | 0.001 | 1.00 | -1297012.00 |
| MET94 | HA | 0.91 | 0.009 | 1.00 | 0.10 |

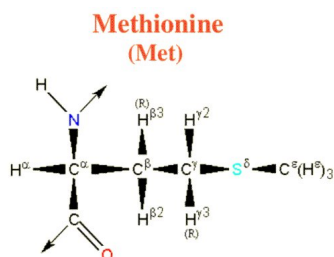
3.94 MET(94)

Figure 84: Image from the BMRB

Residue probability: 0.721

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 179.449 | 176.360 | 2.004 | 0.000 | 0.000 |
| CA 3.94.1 | 58.974 | 56.303 | 4.222 | 0.808 | 1.000 |
| CB 3.94.2 | 31.488 | 33.217 | 4.564 | 0.571 | 1.000 |
| CG 3.94.3 | 32.249 | 32.123 | 4.122 | 1.000 | 1.000 |
| CE 3.94.4 | 16.219 | 17.286 | 5.508 | 0.215 | 1.000 |
| N 3.94.5 | 118.345 | 120.023 | 5.158 | 0.923 | 1.000 |
| HA 3.94.6 | 4.279 | 4.409 | 0.504 | 0.917 | 1.000 |
| HB2 3.94.7 | 2.121 | 2.016 | 0.340 | 0.630 | 1.000 |
| HB3 3.94.8 | 2.032 | 1.978 | 0.359 | 0.629 | 1.000 |
| HG2 3.94.9 | 2.524 | 2.410 | 0.360 | 0.750 | 1.000 |
| HG3 3.94.10 | 2.666 | 2.378 | 0.386 | 0.857 | 1.000 |
| HE 3.94.11 | 2.024 | 1.877 | 0.381 | 0.513 | 1.000 |
| H 3.94.12 | 8.632 | 8.269 | 0.585 | 0.836 | 1.000 |

3.94.1 Detailed Probabilities of MET94CA:

Overall probability: 0.808

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE93 | 0.67 | 1.00 |
| MET94 | 1.00 | 1.00 |
| ASP95 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| I93HA | 1.00 |
| M94HB2 | 1.00 |
| M94HB3 | 1.00 |
| M94HG2 | 1.00 |
| M94HG3 | 1.00 |
| M94H | 1.00 |
| M94HA | 1.00 |
| D95H | 1.00 |
| D95HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE93 | HA | 1.00 | 0.258 | 0.00 | 0.00 |
| ILE93 | HG21 | 0.73 | 0.010 | 1.00 | 0.25 |
| ILE93 | H | 0.91 | 0.009 | 1.00 | 0.10 |
| MET94 | HA | 1.00 | 0.004 | 1.00 | 7.91 |
| MET94 | HB2 | 1.00 | 0.010 | 1.00 | 0.52 |
| MET94 | HB3 | 1.00 | 0.004 | 1.00 | 0.85 |
| MET94 | HG2 | 1.00 | 0.004 | 1.00 | 0.45 |
| MET94 | HG3 | 1.00 | 0.003 | 1.00 | 0.32 |
| MET94 | H | 1.00 | 0.006 | 1.00 | 0.70 |
| MET94 | HE1 | 0.69 | 0.004 | 1.00 | 0.85 |
| ASP95 | HA | 1.00 | 0.035 | 0.50 | 0.00 |
| ASP95 | H | 1.00 | 0.063 | 0.00 | 0.00 |
| ASP95 | HB2 | 0.54 | 0.003 | 1.00 | 0.05 |

3.94.2 Detailed Probabilities of MET94CB:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET94 | 0.58 | 1.00 |
| ASP95 | 0.55 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M94HA | 1.00 |
| M94HB3 | 1.00 |
| M94HG2 | 1.00 |
| M94HG3 | 1.00 |
| M94HE1 | 0.96 |
| M94H | 1.00 |
| M94HB2 | 1.00 |
| D95H | 1.00 |

NOESY contacts detailed probability

3.94 MET(94)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET94 | HA | 1.00 | 0.003 | 1.00 | 0.34 |
| MET94 | HB2 | 1.00 | 0.029 | 1.00 | 28.97 |
| MET94 | HB3 | 1.00 | 0.084 | 0.00 | 0.00 |
| MET94 | HG2 | 1.00 | 0.140 | 0.00 | 0.00 |
| MET94 | HG3 | 1.00 | 0.002 | 1.00 | 0.21 |
| MET94 | HE1 | 0.96 | 0.076 | 0.04 | 0.00 |
| MET94 | H | 1.00 | 0.030 | 1.00 | 0.00 |
| ASP95 | H | 1.00 | 0.039 | 0.10 | 0.00 |
| ASP95 | HA | 0.69 | 0.007 | 1.00 | 1.00 |

3.94.3 Detailed Probabilities of MET94CG:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET94 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M94HA | 1.00 |
| M94HB2 | 1.00 |
| M94HB3 | 1.00 |
| M94HG2 | 1.00 |
| M94HE1 | 1.00 |
| M94H | 1.00 |
| M94HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET94 | HA | 1.00 | 0.002 | 1.00 | 0.17 |
| MET94 | HB2 | 1.00 | 0.006 | 1.00 | 0.39 |
| MET94 | HB3 | 1.00 | 0.012 | 1.00 | 0.60 |
| MET94 | HG2 | 1.00 | 0.002 | 1.00 | 1.86 |
| MET94 | HG3 | 1.00 | 0.002 | 1.00 | 3.04 |
| MET94 | HE1 | 1.00 | 0.004 | 1.00 | 0.60 |
| MET94 | H | 1.00 | 0.006 | 1.00 | 0.27 |

3.94.4 Detailed Probabilities of MET94CE:

Overall probability: 0.215

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET94 | 0.22 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M94HB2 | 0.96 |
| M94HB3 | 0.97 |
| M94HG2 | 1.00 |
| M94HG3 | 1.00 |
| M94HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET94 | HB2 | 0.96 | 0.404 | 0.04 | 0.00 |
| MET94 | HB3 | 0.97 | 0.493 | 0.03 | 0.00 |
| MET94 | HG2 | 1.00 | 0.001 | 1.00 | 0.14 |
| MET94 | HG3 | 1.00 | 0.126 | 0.00 | 0.00 |
| MET94 | HE1 | 1.00 | 0.501 | 0.00 | 0.00 |

3.94.5 Detailed Probabilities of MET94N:

Overall probability: 0.923

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE93 | 1.00 | 1.00 |
| MET94 | 1.00 | 1.00 |
| ASP95 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I93HG12 | 0.97 |
| I93H | 1.00 |
| I93HG21 | 0.98 |
| I93HB | 1.00 |
| I93HA | 1.00 |
| M94HA | 1.00 |
| M94HB2 | 1.00 |
| M94HB3 | 1.00 |
| M94HG2 | 1.00 |
| M94HG3 | 1.00 |
| M94H | 1.00 |
| D95H | 1.00 |

NOESY contacts detailed probability

3.94 MET(94)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE93 | HA | 1.00 | 0.006 | 1.00 | -238315.00 |
| ILE93 | HB | 1.00 | 0.000 | 1.00 | -1062626.00 |
| ILE93 | HG12 | 0.97 | 0.004 | 1.00 | -120159.00 |
| ILE93 | HG21 | 0.98 | 0.008 | 1.00 | -555329.00 |
| ILE93 | H | 1.00 | 0.001 | 1.00 | -1297012.00 |
| MET94 | HA | 1.00 | 0.001 | 1.00 | -1043291.00 |
| MET94 | HB2 | 1.00 | 0.005 | 1.00 | -1348427.00 |
| MET94 | HB3 | 1.00 | 0.004 | 1.00 | -1103036.00 |
| MET94 | HG2 | 1.00 | 0.005 | 1.00 | -892467.00 |
| MET94 | HG3 | 1.00 | 0.003 | 1.00 | -885392.00 |
| MET94 | H | 1.00 | 0.005 | 1.00 | -10772325.00 |
| ASP95 | H | 1.00 | 0.064 | 0.00 | 0.00 |
| ASP95 | HA | 0.85 | 0.004 | 1.00 | -100714.00 |

3.94.6 Detailed Probabilities of MET94HA:

Overall probability: 0.917

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE93 | 0.67 | 1.00 |
| MET94 | 1.00 | 1.00 |
| ASP95 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| I93HA | 1.00 |
| M94HB2 | 1.00 |
| M94HB3 | 1.00 |
| M94HG2 | 1.00 |
| M94HG3 | 1.00 |
| M94H | 1.00 |
| M94HA | 1.00 |
| D95H | 1.00 |
| D95HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE93 | HA | 1.00 | 0.077 | 0.00 | 0.00 |
| ILE93 | HB | 0.89 | 0.002 | 1.00 | 0.05 |
| ILE93 | HG21 | 0.73 | 0.001 | 1.00 | 0.15 |
| MET94 | HA | 1.00 | 0.004 | 1.00 | 7.91 |
| MET94 | HB2 | 1.00 | 0.003 | 1.00 | 0.34 |
| MET94 | HB3 | 1.00 | 0.001 | 1.00 | 0.31 |
| MET94 | HG2 | 1.00 | 0.004 | 1.00 | 0.35 |
| MET94 | HG3 | 1.00 | 0.002 | 1.00 | 0.17 |
| MET94 | H | 1.00 | 0.001 | 1.00 | -1043291.00 |
| ASP95 | HA | 1.00 | 0.017 | 1.00 | 0.26 |
| ASP95 | H | 1.00 | 0.004 | 1.00 | -393660.00 |
| ASP95 | HB2 | 0.54 | 0.012 | 1.00 | 0.07 |

3.94.7 Detailed Probabilities of MET94HB2:

Overall probability: 0.630

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET94 | 0.58 | 1.00 |
| ASP95 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M94HA | 1.00 |
| M94HB3 | 1.00 |
| M94HG2 | 1.00 |
| M94HG3 | 1.00 |
| M94HE1 | 0.96 |
| M94H | 1.00 |
| M94HB2 | 1.00 |
| D95H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET94 | HA | 1.00 | 0.010 | 1.00 | 0.52 |
| MET94 | HB2 | 1.00 | 0.029 | 1.00 | 28.97 |
| MET94 | HB3 | 1.00 | 0.544 | 0.00 | 0.00 |
| MET94 | HG2 | 1.00 | 0.069 | 0.00 | 0.00 |
| MET94 | HG3 | 1.00 | 0.006 | 1.00 | 0.39 |
| MET94 | HE1 | 0.96 | 0.404 | 0.04 | 0.00 |
| MET94 | H | 1.00 | 0.005 | 1.00 | -1348427.00 |
| ASP95 | H | 1.00 | 0.005 | 1.00 | -862560.00 |

3.94.8 Detailed Probabilities of MET94HB3:

Overall probability: 0.629

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET94 | 0.58 | 1.00 |
| ASP95 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M94HA | 1.00 |
| M94HB2 | 1.00 |
| M94HG2 | 1.00 |
| M94HG3 | 1.00 |
| M94HE1 | 0.97 |
| M94H | 1.00 |
| M94HB3 | 1.00 |
| D95H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET94 | HA | 1.00 | 0.004 | 1.00 | 0.85 |
| MET94 | HB2 | 1.00 | 0.084 | 0.00 | 0.00 |
| MET94 | HB3 | 1.00 | 0.633 | 0.00 | 0.00 |
| MET94 | HG2 | 1.00 | 0.020 | 1.00 | 3.95 |
| MET94 | HG3 | 1.00 | 0.012 | 1.00 | 0.60 |
| MET94 | HE1 | 0.97 | 0.493 | 0.03 | 0.00 |
| MET94 | H | 1.00 | 0.004 | 1.00 | -1103036.00 |
| ASP95 | H | 1.00 | 0.006 | 1.00 | -739757.00 |

3.94.9 Detailed Probabilities of MET94HG2:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET94 | 0.71 | 1.00 |
| ASP95 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M94HA | 1.00 |
| M94HB2 | 1.00 |
| M94HB3 | 1.00 |
| M94HG3 | 1.00 |
| M94HE1 | 1.00 |
| M94H | 1.00 |
| M94HG2 | 1.00 |
| D95H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET94 | HA | 1.00 | 0.004 | 1.00 | 0.45 |
| MET94 | HB2 | 1.00 | 0.140 | 0.00 | 0.00 |
| MET94 | HB3 | 1.00 | 0.141 | 0.00 | 0.00 |
| MET94 | HG2 | 1.00 | 0.012 | 1.00 | 6.65 |
| MET94 | HG3 | 1.00 | 0.002 | 1.00 | 1.86 |
| MET94 | HE1 | 1.00 | 0.001 | 1.00 | 0.14 |
| MET94 | H | 1.00 | 0.005 | 1.00 | -892467.00 |
| ASP95 | H | 0.97 | 0.003 | 1.00 | -146235.00 |

3.94.10 Detailed Probabilities of MET94HG3:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET94 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M94HA | 1.00 |
| M94HB2 | 1.00 |
| M94HB3 | 1.00 |
| M94HG2 | 1.00 |
| M94HE1 | 1.00 |
| M94H | 1.00 |
| M94HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET94 | HA | 1.00 | 0.003 | 1.00 | 0.32 |
| MET94 | HB2 | 1.00 | 0.002 | 1.00 | 0.21 |
| MET94 | HB3 | 1.00 | 0.001 | 1.00 | 0.21 |
| MET94 | HG2 | 1.00 | 0.000 | 1.00 | 1.92 |
| MET94 | HG3 | 1.00 | 0.002 | 1.00 | 3.04 |
| MET94 | HE1 | 1.00 | 0.126 | 0.00 | 0.00 |
| MET94 | H | 1.00 | 0.003 | 1.00 | -885392.00 |

3.94.11 Detailed Probabilities of MET94HE1:

Overall probability: 0.513

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET94 | 0.51 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M94HB2 | 0.96 |
| M94HB3 | 0.97 |
| M94HG2 | 1.00 |
| M94HG3 | 1.00 |
| M94HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET94 | HB2 | 0.96 | 0.076 | 0.04 | 0.00 |
| MET94 | HB3 | 0.97 | 0.641 | 0.03 | 0.00 |
| MET94 | HG2 | 1.00 | 0.028 | 1.00 | 3.95 |
| MET94 | HG3 | 1.00 | 0.004 | 1.00 | 0.60 |
| MET94 | HE1 | 1.00 | 0.501 | 0.00 | 0.00 |
| MET94 | HA | 0.67 | 0.004 | 1.00 | 0.85 |

3.94.12 Detailed Probabilities of MET94H:

Overall probability: 0.836

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ILE93 | 0.81 | 1.00 |
| MET94 | 1.00 | 1.00 |
| ASP95 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| I93HG12 | 0.97 |
| I93H | 1.00 |
| I93HG21 | 0.98 |
| I93HB | 1.00 |
| I93HA | 1.00 |
| M94HA | 1.00 |
| M94HB2 | 1.00 |
| M94HB3 | 1.00 |
| M94HG2 | 1.00 |
| M94HG3 | 1.00 |
| M94H | 1.00 |
| D95H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ILE93 | HA | 1.00 | 0.005 | 1.00 | 0.22 |
| ILE93 | HB | 1.00 | 0.007 | 1.00 | 0.30 |
| ILE93 | HG12 | 0.97 | 0.382 | 0.03 | 0.00 |
| ILE93 | HG21 | 0.98 | 0.001 | 1.00 | 0.38 |
| ILE93 | H | 1.00 | 0.006 | 1.00 | -923181.00 |
| MET94 | HA | 1.00 | 0.006 | 1.00 | 0.70 |
| MET94 | HB2 | 1.00 | 0.030 | 1.00 | 0.00 |
| MET94 | HB3 | 1.00 | 0.012 | 1.00 | 0.27 |
| MET94 | HG2 | 1.00 | 0.008 | 1.00 | 0.32 |
| MET94 | HG3 | 1.00 | 0.006 | 1.00 | 0.27 |
| MET94 | H | 1.00 | 0.005 | 1.00 | -10772325.00 |
| ASP95 | H | 1.00 | 0.069 | 0.00 | 0.00 |

3.95 ASP(95)

Figure 85: Image from the BMRB

Residue probability: 0.774

Residue probability confidence: 0.893

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 178.903 | 176.463 | 2.348 | 0.000 | 0.000 |
| CA 3.95.1 | 57.053 | 54.786 | 4.266 | 0.714 | 0.875 |
| CB 3.95.2 | 40.075 | 40.949 | 3.070 | 0.833 | 0.833 |
| N 3.95.3 | 120.052 | 120.550 | 5.690 | 0.909 | 1.000 |
| HD2 | NA | – | – | 0.000 | 0.000 |
| HA 3.95.4 | 4.412 | 4.587 | 0.329 | 0.650 | 0.875 |
| HB2 3.95.5 | 2.861 | 2.708 | 0.282 | 1.000 | 0.833 |
| HB3 3.95.6 | 2.659 | 2.654 | 0.285 | 1.000 | 0.833 |
| H 3.95.7 | 8.701 | 8.304 | 1.027 | 0.313 | 1.000 |

3.95.1 Detailed Probabilities of ASP95CA:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET94 | 1.00 | 1.00 |
| ASP95 | 0.75 | 0.80 |
| PHE96 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M94HA | 1.00 |
| D95HD2 | 1.00 |
| D95HB2 | 1.00 |
| D95HB3 | 1.00 |
| D95H | 1.00 |
| D95HA | 1.00 |
| F96HA | 1.00 |
| F96H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET94 | HA | 1.00 | 0.017 | 1.00 | 0.26 |
| ASP95 | HA | 1.00 | 0.150 | 0.00 | 0.00 |
| ASP95 | HB2 | 1.00 | 0.004 | 1.00 | 1.06 |
| ASP95 | HB3 | 1.00 | 0.008 | 1.00 | 1.25 |
| ASP95 | H | 1.00 | 0.000 | 1.00 | 0.72 |
| PHE96 | HA | 1.00 | 0.078 | 0.00 | 0.00 |
| PHE96 | H | 1.00 | 0.002 | 1.00 | 0.26 |

3.95.2 Detailed Probabilities of ASP95CB:

Overall probability: 0.833

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP95 | 0.75 | 0.80 |
| PHE96 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D95HD2 | 1.00 |
| D95HA | 1.00 |
| D95HB3 | 1.00 |
| D95H | 1.00 |
| D95HB2 | 1.00 |
| F96H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP95 | HA | 1.00 | 0.000 | 1.00 | 0.92 |
| ASP95 | HB2 | 1.00 | 0.002 | 1.00 | 5.06 |
| ASP95 | HB3 | 1.00 | 0.007 | 1.00 | 5.29 |
| ASP95 | H | 1.00 | 0.088 | 0.00 | 0.00 |
| PHE96 | H | 1.00 | 0.004 | 1.00 | 0.38 |
| PHE96 | HA | 0.51 | 0.021 | 1.00 | 0.08 |

3.95.3 Detailed Probabilities of ASP95N:

Overall probability: 0.909

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET94 | 0.83 | 1.00 |
| ASP95 | 1.00 | 1.00 |
| PHE96 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M94H | 1.00 |
| M94HG2 | 0.97 |
| M94HB3 | 1.00 |
| M94HB2 | 1.00 |
| M94HA | 1.00 |
| D95HA | 1.00 |
| D95HB2 | 1.00 |
| D95HB3 | 1.00 |
| D95H | 1.00 |
| F96H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET94 | HA | 1.00 | 0.004 | 1.00 | -393660.00 |
| MET94 | HB2 | 1.00 | 0.005 | 1.00 | -862560.00 |
| MET94 | HB3 | 1.00 | 0.006 | 1.00 | -739757.00 |
| MET94 | HG2 | 0.97 | 0.003 | 1.00 | -146235.00 |
| MET94 | H | 1.00 | 0.069 | 0.00 | 0.00 |
| MET94 | HG3 | 0.95 | 0.010 | 1.00 | -1385790.00 |
| ASP95 | HA | 1.00 | 0.001 | 1.00 | -1238841.00 |
| ASP95 | HB2 | 1.00 | 0.004 | 1.00 | -2313457.00 |
| ASP95 | HB3 | 1.00 | 0.003 | 1.00 | -1385790.00 |
| ASP95 | H | 1.00 | 0.000 | 1.00 | -13223265.00 |
| PHE96 | H | 1.00 | 0.004 | 1.00 | -1273724.00 |

3.95.4 Detailed Probabilities of ASP95HA:

Overall probability: 0.650

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET94 | 0.87 | 1.00 |
| ASP95 | 0.50 | 0.80 |
| PHE96 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M94HA | 1.00 |
| D95HD2 | 1.00 |
| D95HB2 | 1.00 |
| D95HB3 | 1.00 |
| D95H | 1.00 |
| D95HA | 1.00 |
| F96HA | 1.00 |
| F96H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET94 | HA | 1.00 | 0.035 | 0.50 | 0.00 |
| MET94 | HB2 | 0.69 | 0.007 | 1.00 | 1.00 |
| MET94 | HB3 | 0.79 | 0.003 | 1.00 | 0.09 |
| MET94 | H | 0.85 | 0.004 | 1.00 | -100714.00 |
| ASP95 | HA | 1.00 | 0.150 | 0.00 | 0.00 |
| ASP95 | HB2 | 1.00 | 0.000 | 1.00 | 0.92 |
| ASP95 | HB3 | 1.00 | 0.389 | 0.00 | 0.00 |
| ASP95 | H | 1.00 | 0.001 | 1.00 | -1238841.00 |
| PHE96 | HA | 1.00 | 0.208 | 0.00 | 0.00 |
| PHE96 | H | 1.00 | 0.005 | 1.00 | -292371.00 |

3.95.5 Detailed Probabilities of ASP95HB2:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP95 | 1.00 | 0.80 |
| PHE96 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D95HD2 | 1.00 |
| D95HA | 1.00 |
| D95HB3 | 1.00 |
| D95H | 1.00 |
| D95HB2 | 1.00 |
| F96H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP95 | HA | 1.00 | 0.004 | 1.00 | 1.06 |
| ASP95 | HB2 | 1.00 | 0.002 | 1.00 | 5.06 |
| ASP95 | HB3 | 1.00 | 0.003 | 1.00 | 5.64 |
| ASP95 | H | 1.00 | 0.004 | 1.00 | -2313457.00 |
| PHE96 | H | 1.00 | 0.003 | 1.00 | -776238.00 |

3.95.6 Detailed Probabilities of ASP95HB3:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP95 | 1.00 | 0.80 |
| PHE96 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D95HD2 | 1.00 |
| D95HA | 1.00 |
| D95HB2 | 1.00 |
| D95H | 1.00 |
| D95HB3 | 1.00 |
| F96H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP95 | HA | 1.00 | 0.008 | 1.00 | 1.25 |
| ASP95 | HB2 | 1.00 | 0.007 | 1.00 | 5.29 |
| ASP95 | HB3 | 1.00 | 0.001 | 1.00 | 11.11 |
| ASP95 | H | 1.00 | 0.003 | 1.00 | -1385790.00 |
| PHE96 | H | 1.00 | 0.003 | 1.00 | -607798.00 |
| PHE96 | HA | 0.83 | 0.006 | 1.00 | 0.09 |

3.95.7 Detailed Probabilities of ASP95H:

Overall probability: 0.313

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| MET94 | 0.03 | 1.00 |
| ASP95 | 0.50 | 1.00 |
| PHE96 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| M94H | 1.00 |
| M94HG2 | 0.97 |
| M94HB3 | 1.00 |
| M94HB2 | 1.00 |
| M94HA | 1.00 |
| D95HA | 1.00 |
| D95HB2 | 1.00 |
| D95HB3 | 1.00 |
| D95H | 1.00 |
| F96H | 1.00 |

NOESY contacts detailed probability

3.95 ASP(95)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| MET94 | HA | 1.00 | 0.063 | 0.00 | 0.00 |
| MET94 | HB2 | 1.00 | 0.039 | 0.10 | 0.00 |
| MET94 | HB3 | 1.00 | 0.057 | 0.00 | 0.00 |
| MET94 | HG2 | 0.97 | 0.061 | 0.03 | 0.00 |
| MET94 | H | 1.00 | 0.064 | 0.00 | 0.00 |
| ASP95 | HA | 1.00 | 0.000 | 1.00 | 0.72 |
| ASP95 | HB2 | 1.00 | 0.088 | 0.00 | 0.00 |
| ASP95 | HB3 | 1.00 | 0.131 | 0.00 | 0.00 |
| ASP95 | H | 1.00 | 0.000 | 1.00 | -13223265.00 |
| PHE96 | H | 1.00 | 0.004 | 1.00 | -1016419.00 |

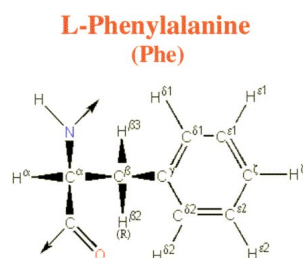
3.96 PHE(96)

Figure 86: Image from the BMRB

Residue probability: 0.864

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 180.567 | 175.508 | 2.010 | 0.000 | 0.000 |
| CA 3.96.1 | 61.997 | 58.245 | 3.808 | 0.760 | 1.000 |
| CB 3.96.2 | 39.421 | 40.078 | 3.616 | 0.889 | 1.000 |
| CD1 3.96.3 | 131.323 | 131.234 | 9.579 | 0.889 | 1.000 |
| CD2 3.96.4 | 131.330 | 131.352 | 9.581 | 0.891 | 1.000 |
| CE1 3.96.5 | 131.473 | 130.599 | 3.219 | 1.000 | 1.000 |
| CE2 3.96.6 | 131.553 | 130.633 | 2.839 | 0.857 | 1.000 |
| CZ 3.96.7 | 131.124 | 129.042 | 3.448 | 0.600 | 1.000 |
| N 3.96.8 | 120.516 | 120.315 | 4.931 | 1.000 | 1.000 |
| HA 3.96.9 | 4.060 | 4.625 | 1.237 | 0.840 | 1.000 |
| HB2 3.96.10 | 3.252 | 2.980 | 0.399 | 0.625 | 1.000 |
| HB3 3.96.11 | 2.945 | 2.916 | 0.434 | 0.889 | 1.000 |
| HD1 3.96.12 | 6.616 | 7.037 | 0.347 | 1.000 | 1.000 |
| HD2 3.96.13 | 6.616 | 7.022 | 0.417 | 1.000 | 1.000 |
| HE1 3.96.14 | 6.805 | 7.046 | 0.417 | 0.857 | 1.000 |
| HE2 3.96.15 | 6.805 | 7.043 | 0.400 | 0.857 | 1.000 |
| HZ 3.96.16 | 6.968 | 6.984 | 1.598 | 1.000 | 1.000 |
| H 3.96.17 | 8.235 | 8.375 | 0.710 | 0.729 | 1.000 |

3.96.1 Detailed Probabilities of PHE96CA:

Overall probability: 0.760

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP95 | 0.50 | 1.00 |
| PHE96 | 1.00 | 1.00 |
| PHE97 | 0.30 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D95HA | 1.00 |
| F96HB2 | 1.00 |
| F96HB3 | 1.00 |
| F96HD1 | 1.00 |
| F96HD2 | 1.00 |
| F96H | 1.00 |
| F96HA | 1.00 |
| F97HA | 1.00 |
| F97H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP95 | HA | 1.00 | 0.208 | 0.00 | 0.00 |
| ASP95 | HB3 | 0.83 | 0.006 | 1.00 | 0.09 |
| PHE96 | HA | 1.00 | 0.001 | 1.00 | 6.63 |
| PHE96 | HB2 | 1.00 | 0.004 | 1.00 | 0.91 |
| PHE96 | HB3 | 1.00 | 0.001 | 1.00 | 0.49 |
| PHE96 | HD1 | 1.00 | 0.005 | 1.00 | 0.61 |
| PHE96 | HD2 | 1.00 | 0.005 | 1.00 | 0.61 |
| PHE96 | H | 1.00 | 0.002 | 1.00 | 0.57 |
| PHE97 | HA | 1.00 | 0.034 | 0.60 | 0.00 |
| PHE97 | H | 1.00 | 0.387 | 0.00 | 0.00 |

3.96.2 Detailed Probabilities of PHE96CB:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE96 | 0.88 | 1.00 |
| PHE97 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F96HA | 1.00 |
| F96HB3 | 1.00 |
| F96HD1 | 1.00 |
| F96HD2 | 1.00 |
| F96HE2 | 1.00 |
| F96H | 1.00 |
| F96HB2 | 1.00 |
| F97H | 1.00 |

NOESY contacts detailed probability

3.96 PHE(96)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE96 | HA | 1.00 | 0.002 | 1.00 | 0.60 |
| PHE96 | HB2 | 1.00 | 0.274 | 0.00 | 0.00 |
| PHE96 | HB3 | 1.00 | 0.002 | 1.00 | 1.71 |
| PHE96 | HD1 | 1.00 | 0.004 | 1.00 | 0.59 |
| PHE96 | HD2 | 1.00 | 0.004 | 1.00 | 0.59 |
| PHE96 | HE2 | 1.00 | 0.009 | 1.00 | 0.08 |
| PHE96 | H | 1.00 | 0.004 | 1.00 | 0.65 |
| PHE96 | HE1 | 0.90 | 0.009 | 1.00 | 0.08 |
| PHE97 | H | 1.00 | 0.006 | 1.00 | 0.25 |

3.96.3 Detailed Probabilities of PHE96CD1:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE96 | 0.89 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F96HA | 1.00 |
| F96HB2 | 1.00 |
| F96HB3 | 1.00 |
| F96HD2 | 1.00 |
| F96HE1 | 1.00 |
| F96HE2 | 1.00 |
| F96HZ | 1.00 |
| F96H | 1.00 |
| F96HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE96 | HA | 1.00 | 0.003 | 1.00 | 0.10 |
| PHE96 | HB2 | 1.00 | 0.004 | 1.00 | 0.12 |
| PHE96 | HB3 | 1.00 | 0.005 | 1.00 | 0.49 |
| PHE96 | HD1 | 1.00 | 0.005 | 1.00 | 1.63 |
| PHE96 | HD2 | 1.00 | 0.005 | 1.00 | 1.63 |
| PHE96 | HE1 | 1.00 | 0.004 | 1.00 | 1.66 |
| PHE96 | HE2 | 1.00 | 0.004 | 1.00 | 1.66 |
| PHE96 | HZ | 1.00 | 0.010 | 1.00 | 0.25 |
| PHE96 | H | 1.00 | 0.391 | 0.00 | 0.00 |

3.96.4 Detailed Probabilities of PHE96CD2:

Overall probability: 0.891

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE96 | 0.89 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F96HA | 1.00 |
| F96HB2 | 1.00 |
| F96HB3 | 1.00 |
| F96HD1 | 1.00 |
| F96HE1 | 1.00 |
| F96HE2 | 1.00 |
| F96HZ | 1.00 |
| F96H | 0.99 |
| F96HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE96 | HA | 1.00 | 0.003 | 1.00 | 0.10 |
| PHE96 | HB2 | 1.00 | 0.004 | 1.00 | 0.12 |
| PHE96 | HB3 | 1.00 | 0.005 | 1.00 | 0.49 |
| PHE96 | HD1 | 1.00 | 0.005 | 1.00 | 1.63 |
| PHE96 | HD2 | 1.00 | 0.005 | 1.00 | 1.63 |
| PHE96 | HE1 | 1.00 | 0.004 | 1.00 | 1.66 |
| PHE96 | HE2 | 1.00 | 0.004 | 1.00 | 1.66 |
| PHE96 | HZ | 1.00 | 0.010 | 1.00 | 0.25 |
| PHE96 | H | 0.99 | 0.391 | 0.01 | 0.00 |

3.96.5 Detailed Probabilities of PHE96CE1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE96 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F96HD1 | 1.00 |
| F96HD2 | 1.00 |
| F96HE2 | 1.00 |
| F96HZ | 1.00 |
| F96HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE96 | HD1 | 1.00 | 0.000 | 1.00 | 0.28 |
| PHE96 | HD2 | 1.00 | 0.000 | 1.00 | 0.28 |
| PHE96 | HE1 | 1.00 | 0.002 | 1.00 | 4.22 |
| PHE96 | HE2 | 1.00 | 0.002 | 1.00 | 4.22 |
| PHE96 | HZ | 1.00 | 0.005 | 1.00 | 0.84 |
| PHE96 | HB3 | 0.89 | 0.000 | 1.00 | 0.15 |

3.96.6 Detailed Probabilities of PHE96CE2:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE96 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F96HB2 | 1.00 |
| F96HB3 | 1.00 |
| F96HD1 | 1.00 |
| F96HD2 | 1.00 |
| F96HE1 | 1.00 |
| F96HZ | 1.00 |
| F96HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE96 | HB2 | 1.00 | 0.307 | 0.00 | 0.00 |
| PHE96 | HB3 | 1.00 | 0.000 | 1.00 | 0.15 |
| PHE96 | HD1 | 1.00 | 0.000 | 1.00 | 0.28 |
| PHE96 | HD2 | 1.00 | 0.000 | 1.00 | 0.28 |
| PHE96 | HE1 | 1.00 | 0.002 | 1.00 | 4.22 |
| PHE96 | HE2 | 1.00 | 0.002 | 1.00 | 4.22 |
| PHE96 | HZ | 1.00 | 0.005 | 1.00 | 0.84 |

3.96.7 Detailed Probabilities of PHE96CZ:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE96 | 0.60 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F96HD1 | 1.00 |
| F96HD2 | 1.00 |
| F96HE1 | 1.00 |
| F96HE2 | 1.00 |
| F96HZ | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE96 | HD1 | 1.00 | 0.011 | 1.00 | 2.37 |
| PHE96 | HD2 | 1.00 | 0.011 | 1.00 | 2.37 |
| PHE96 | HE1 | 1.00 | 0.152 | 0.00 | 0.00 |
| PHE96 | HE2 | 1.00 | 0.152 | 0.00 | 0.00 |
| PHE96 | HZ | 1.00 | 0.010 | 1.00 | 28.23 |

3.96.8 Detailed Probabilities of PHE96N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP95 | 1.00 | 1.00 |
| PHE96 | 1.00 | 1.00 |
| PHE97 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D95HB2 | 1.00 |
| D95HB3 | 1.00 |
| D95H | 1.00 |
| D95HA | 1.00 |
| F96HA | 1.00 |
| F96HB2 | 1.00 |
| F96HB3 | 1.00 |
| F96HD1 | 1.00 |
| F96HD2 | 0.99 |
| F96H | 1.00 |
| F97H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP95 | HA | 1.00 | 0.005 | 1.00 | -292371.00 |
| ASP95 | HB2 | 1.00 | 0.003 | 1.00 | -776238.00 |
| ASP95 | HB3 | 1.00 | 0.003 | 1.00 | -607798.00 |
| ASP95 | H | 1.00 | 0.004 | 1.00 | -1016419.00 |
| PHE96 | HA | 1.00 | 0.003 | 1.00 | -782605.00 |
| PHE96 | HB2 | 1.00 | 0.003 | 1.00 | -1237267.00 |
| PHE96 | HB3 | 1.00 | 0.005 | 1.00 | -1233295.00 |
| PHE96 | HD1 | 1.00 | 0.005 | 1.00 | -314962.00 |
| PHE96 | HD2 | 0.99 | 0.005 | 1.00 | -314962.00 |
| PHE96 | H | 1.00 | 0.003 | 1.00 | -8574048.00 |
| PHE97 | H | 1.00 | 0.016 | 1.00 | -854700.00 |
| PHE97 | HB2 | 0.56 | 0.012 | 1.00 | -132639.00 |

3.96.9 Detailed Probabilities of PHE96HA:

Overall probability: 0.840

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP95 | 0.50 | 1.00 |
| PHE96 | 1.00 | 1.00 |
| PHE97 | 0.70 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D95HA | 1.00 |
| F96HB2 | 1.00 |
| F96HB3 | 1.00 |
| F96HD1 | 1.00 |
| F96HD2 | 1.00 |
| F96H | 1.00 |
| F96HA | 1.00 |
| F97HA | 1.00 |
| F97H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP95 | HA | 1.00 | 0.078 | 0.00 | 0.00 |
| ASP95 | HB2 | 0.51 | 0.021 | 1.00 | 0.08 |
| PHE96 | HA | 1.00 | 0.001 | 1.00 | 6.63 |
| PHE96 | HB2 | 1.00 | 0.002 | 1.00 | 0.60 |
| PHE96 | HB3 | 1.00 | 0.000 | 1.00 | 0.38 |
| PHE96 | HD1 | 1.00 | 0.003 | 1.00 | 0.10 |
| PHE96 | HD2 | 1.00 | 0.003 | 1.00 | 0.10 |
| PHE96 | H | 1.00 | 0.003 | 1.00 | -782605.00 |
| PHE97 | HA | 1.00 | 0.035 | 0.50 | 0.00 |
| PHE97 | H | 1.00 | 0.031 | 0.90 | 0.00 |

3.96.10 Detailed Probabilities of PHE96HB2:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE96 | 0.71 | 1.00 |
| PHE97 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F96HA | 1.00 |
| F96HB3 | 1.00 |
| F96HD1 | 1.00 |
| F96HD2 | 1.00 |
| F96HE2 | 1.00 |
| F96H | 1.00 |
| F96HB2 | 1.00 |
| F97H | 1.00 |

NOESY contacts detailed probability

3.96 PHE(96)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE96 | HA | 1.00 | 0.004 | 1.00 | 0.91 |
| PHE96 | HB2 | 1.00 | 0.274 | 0.00 | 0.00 |
| PHE96 | HB3 | 1.00 | 0.002 | 1.00 | 1.59 |
| PHE96 | HD1 | 1.00 | 0.004 | 1.00 | 0.12 |
| PHE96 | HD2 | 1.00 | 0.004 | 1.00 | 0.12 |
| PHE96 | HE2 | 1.00 | 0.307 | 0.00 | 0.00 |
| PHE96 | H | 1.00 | 0.003 | 1.00 | -1237267.00 |
| PHE97 | H | 1.00 | 0.066 | 0.00 | 0.00 |

3.96.11 Detailed Probabilities of PHE96HB3:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE96 | 0.88 | 1.00 |
| PHE97 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F96HA | 1.00 |
| F96HB2 | 1.00 |
| F96HD1 | 1.00 |
| F96HD2 | 1.00 |
| F96HE2 | 1.00 |
| F96H | 1.00 |
| F96HB3 | 1.00 |
| F97H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE96 | HA | 1.00 | 0.001 | 1.00 | 0.49 |
| PHE96 | HB2 | 1.00 | 0.002 | 1.00 | 1.71 |
| PHE96 | HB3 | 1.00 | 0.305 | 0.00 | 0.00 |
| PHE96 | HD1 | 1.00 | 0.005 | 1.00 | 0.49 |
| PHE96 | HD2 | 1.00 | 0.005 | 1.00 | 0.49 |
| PHE96 | HE2 | 1.00 | 0.000 | 1.00 | 0.15 |
| PHE96 | H | 1.00 | 0.005 | 1.00 | -1233295.00 |
| PHE96 | HE1 | 0.89 | 0.000 | 1.00 | 0.15 |
| PHE97 | H | 1.00 | 0.007 | 1.00 | -823040.00 |

3.96.12 Detailed Probabilities of PHE96HD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE96 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F96HA | 1.00 |
| F96HB2 | 1.00 |
| F96HB3 | 1.00 |
| F96HD2 | 1.00 |
| F96HE1 | 1.00 |
| F96HE2 | 1.00 |
| F96HZ | 1.00 |
| F96H | 1.00 |
| F96HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE96 | HA | 1.00 | 0.005 | 1.00 | 0.61 |
| PHE96 | HB2 | 1.00 | 0.004 | 1.00 | 0.59 |
| PHE96 | HB3 | 1.00 | 0.003 | 1.00 | 0.53 |
| PHE96 | HD1 | 1.00 | 0.005 | 1.00 | 1.63 |
| PHE96 | HD2 | 1.00 | 0.005 | 1.00 | 1.63 |
| PHE96 | HE1 | 1.00 | 0.000 | 1.00 | 0.28 |
| PHE96 | HE2 | 1.00 | 0.000 | 1.00 | 0.28 |
| PHE96 | HZ | 1.00 | 0.011 | 1.00 | 2.37 |
| PHE96 | H | 1.00 | 0.005 | 1.00 | -314962.00 |

3.96.13 Detailed Probabilities of PHE96HD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE96 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F96HA | 1.00 |
| F96HB2 | 1.00 |
| F96HB3 | 1.00 |
| F96HD1 | 1.00 |
| F96HE1 | 1.00 |
| F96HE2 | 1.00 |
| F96HZ | 1.00 |
| F96H | 0.99 |
| F96HD2 | 1.00 |

NOESY contacts detailed probability

3.96 PHE(96)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE96 | HA | 1.00 | 0.005 | 1.00 | 0.61 |
| PHE96 | HB2 | 1.00 | 0.004 | 1.00 | 0.59 |
| PHE96 | HB3 | 1.00 | 0.003 | 1.00 | 0.53 |
| PHE96 | HD1 | 1.00 | 0.005 | 1.00 | 1.63 |
| PHE96 | HD2 | 1.00 | 0.005 | 1.00 | 1.63 |
| PHE96 | HE1 | 1.00 | 0.000 | 1.00 | 0.28 |
| PHE96 | HE2 | 1.00 | 0.000 | 1.00 | 0.28 |
| PHE96 | HZ | 1.00 | 0.011 | 1.00 | 2.37 |
| PHE96 | H | 0.99 | 0.005 | 1.00 | -314962.00 |

3.96.14 Detailed Probabilities of PHE96HE1:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE96 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F96HD1 | 1.00 |
| F96HD2 | 1.00 |
| F96HE2 | 1.00 |
| F96HZ | 1.00 |
| F96HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE96 | HD1 | 1.00 | 0.004 | 1.00 | 1.66 |
| PHE96 | HD2 | 1.00 | 0.004 | 1.00 | 1.66 |
| PHE96 | HE1 | 1.00 | 0.002 | 1.00 | 4.22 |
| PHE96 | HE2 | 1.00 | 0.002 | 1.00 | 4.22 |
| PHE96 | HZ | 1.00 | 0.152 | 0.00 | 0.00 |
| PHE96 | HB2 | 0.90 | 0.009 | 1.00 | 0.08 |
| PHE96 | HB3 | 0.89 | 0.015 | 1.00 | 0.09 |

3.96.15 Detailed Probabilities of PHE96HE2:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE96 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F96HB2 | 1.00 |
| F96HB3 | 1.00 |
| F96HD1 | 1.00 |
| F96HD2 | 1.00 |
| F96HE1 | 1.00 |
| F96HZ | 1.00 |
| F96HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE96 | HB2 | 1.00 | 0.009 | 1.00 | 0.08 |
| PHE96 | HB3 | 1.00 | 0.015 | 1.00 | 0.09 |
| PHE96 | HD1 | 1.00 | 0.004 | 1.00 | 1.66 |
| PHE96 | HD2 | 1.00 | 0.004 | 1.00 | 1.66 |
| PHE96 | HE1 | 1.00 | 0.002 | 1.00 | 4.22 |
| PHE96 | HE2 | 1.00 | 0.002 | 1.00 | 4.22 |
| PHE96 | HZ | 1.00 | 0.152 | 0.00 | 0.00 |

3.96.16 Detailed Probabilities of PHE96HZ:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE96 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F96HD1 | 1.00 |
| F96HD2 | 1.00 |
| F96HE1 | 1.00 |
| F96HE2 | 1.00 |
| F96HZ | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE96 | HD1 | 1.00 | 0.010 | 1.00 | 0.25 |
| PHE96 | HD2 | 1.00 | 0.010 | 1.00 | 0.25 |
| PHE96 | HE1 | 1.00 | 0.005 | 1.00 | 0.84 |
| PHE96 | HE2 | 1.00 | 0.005 | 1.00 | 0.84 |
| PHE96 | HZ | 1.00 | 0.010 | 1.00 | 28.23 |

3.96.17 Detailed Probabilities of PHE96H:

Overall probability: 0.729

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ASP95 | 0.75 | 1.00 |
| PHE96 | 0.67 | 1.00 |
| PHE97 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| D95HB2 | 1.00 |
| D95HB3 | 1.00 |
| D95H | 1.00 |
| D95HA | 1.00 |
| F96HA | 1.00 |
| F96HB2 | 1.00 |
| F96HB3 | 1.00 |
| F96HD1 | 1.00 |
| F96HD2 | 0.99 |
| F96H | 1.00 |
| F97H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ASP95 | HA | 1.00 | 0.002 | 1.00 | 0.26 |
| ASP95 | HB2 | 1.00 | 0.004 | 1.00 | 0.38 |
| ASP95 | HB3 | 1.00 | 0.335 | 0.00 | 0.00 |
| ASP95 | H | 1.00 | 0.004 | 1.00 | -1273724.00 |
| PHE96 | HA | 1.00 | 0.002 | 1.00 | 0.57 |
| PHE96 | HB2 | 1.00 | 0.004 | 1.00 | 0.65 |
| PHE96 | HB3 | 1.00 | 0.005 | 1.00 | 0.61 |
| PHE96 | HD1 | 1.00 | 0.391 | 0.00 | 0.00 |
| PHE96 | HD2 | 0.99 | 0.391 | 0.01 | 0.00 |
| PHE96 | H | 1.00 | 0.003 | 1.00 | -8574048.00 |
| PHE97 | H | 1.00 | 0.003 | 1.00 | -876987.00 |

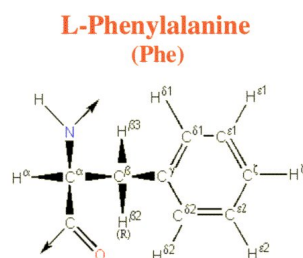
3.97 PHE(97)

Figure 87: Image from the BMRB

Residue probability: 0.787

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 177.057 | 175.508 | 2.010 | 0.000 | 0.000 |
| CA 3.97.1 | 62.385 | 58.245 | 3.808 | 0.650 | 1.000 |
| CB 3.97.2 | 37.867 | 40.078 | 3.616 | 1.000 | 1.000 |
| CD1 3.97.3 | 131.764 | 131.234 | 9.579 | 1.000 | 1.000 |
| CD2 3.97.4 | 131.904 | 131.352 | 9.581 | 1.000 | 1.000 |
| CE1 3.97.5 | 130.744 | 130.599 | 3.219 | 0.400 | 1.000 |
| CE2 3.97.6 | 130.815 | 130.633 | 2.839 | 0.286 | 1.000 |
| CZ 3.97.7 | 129.110 | 129.042 | 3.448 | 1.000 | 1.000 |
| N 3.97.8 | 121.200 | 120.315 | 4.931 | 0.915 | 1.000 |
| HA 3.97.9 | 4.025 | 4.625 | 1.237 | 0.853 | 1.000 |
| HB2 3.97.10 | 3.032 | 2.980 | 0.399 | 0.875 | 1.000 |
| HB3 3.97.11 | 3.182 | 2.916 | 0.434 | 0.875 | 1.000 |
| HD1 3.97.12 | 7.579 | 7.037 | 0.347 | 0.889 | 1.000 |
| HD2 3.97.13 | 7.579 | 7.022 | 0.417 | 0.889 | 1.000 |
| HE1 3.97.14 | 7.217 | 7.046 | 0.417 | 0.714 | 1.000 |
| HE2 3.97.15 | 7.217 | 7.043 | 0.400 | 0.572 | 1.000 |
| HZ 3.97.16 | 7.002 | 6.984 | 1.598 | 0.600 | 1.000 |
| H 3.97.17 | 8.624 | 8.375 | 0.710 | 0.857 | 1.000 |

3.97.1 Detailed Probabilities of PHE97CA:

Overall probability: 0.650

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE96 | 0.50 | 1.00 |
| PHE97 | 0.71 | 1.00 |
| ALA98 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F96HA | 1.00 |
| F97HB2 | 1.00 |
| F97HB3 | 1.00 |
| F97HD1 | 1.00 |
| F97HD2 | 1.00 |
| F97H | 1.00 |
| F97HA | 1.00 |
| A98HA | 1.00 |
| A98H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE96 | HA | 1.00 | 0.035 | 0.50 | 0.00 |
| PHE97 | HA | 1.00 | 0.000 | 1.00 | 6.88 |
| PHE97 | HB2 | 1.00 | 0.010 | 1.00 | 0.43 |
| PHE97 | HB3 | 1.00 | 0.000 | 1.00 | 0.63 |
| PHE97 | HD1 | 1.00 | 0.292 | 0.00 | 0.00 |
| PHE97 | HD2 | 1.00 | 0.292 | 0.00 | 0.00 |
| PHE97 | H | 1.00 | 0.007 | 1.00 | 0.46 |
| PHE97 | HE1 | 0.74 | 0.009 | 1.00 | 0.12 |
| ALA98 | HA | 1.00 | 0.043 | 0.00 | 0.00 |
| ALA98 | H | 1.00 | 0.002 | 1.00 | 0.17 |

3.97.2 Detailed Probabilities of PHE97CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE97 | 1.00 | 1.00 |
| ALA98 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F97HA | 1.00 |
| F97HB3 | 1.00 |
| F97HD1 | 1.00 |
| F97HD2 | 1.00 |
| F97HE2 | 1.00 |
| F97H | 1.00 |
| F97HB2 | 1.00 |
| A98H | 1.00 |

NOESY contacts detailed probability

3.97 PHE(97)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE97 | HA | 1.00 | 0.014 | 1.00 | 0.45 |
| PHE97 | HB2 | 1.00 | 0.004 | 1.00 | 2.08 |
| PHE97 | HB3 | 1.00 | 0.009 | 1.00 | 2.17 |
| PHE97 | HD1 | 1.00 | 0.005 | 1.00 | 0.33 |
| PHE97 | HD2 | 1.00 | 0.005 | 1.00 | 0.33 |
| PHE97 | HE2 | 1.00 | 0.009 | 1.00 | 0.08 |
| PHE97 | H | 1.00 | 0.007 | 1.00 | 0.45 |
| PHE97 | HE1 | 0.90 | 0.009 | 1.00 | 0.08 |
| ALA98 | H | 1.00 | 0.002 | 1.00 | 0.13 |

3.97.3 Detailed Probabilities of PHE97CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE97 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F97HA | 1.00 |
| F97HB2 | 1.00 |
| F97HB3 | 1.00 |
| F97HD2 | 1.00 |
| F97HE1 | 1.00 |
| F97HE2 | 1.00 |
| F97HZ | 1.00 |
| F97H | 1.00 |
| F97HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE97 | HA | 1.00 | 0.002 | 1.00 | 0.58 |
| PHE97 | HB2 | 1.00 | 0.006 | 1.00 | 0.12 |
| PHE97 | HB3 | 1.00 | 0.000 | 1.00 | 0.76 |
| PHE97 | HD1 | 1.00 | 0.003 | 1.00 | 4.75 |
| PHE97 | HD2 | 1.00 | 0.003 | 1.00 | 4.75 |
| PHE97 | HE1 | 1.00 | 0.001 | 1.00 | 0.58 |
| PHE97 | HE2 | 1.00 | 0.001 | 1.00 | 0.58 |
| PHE97 | HZ | 1.00 | 0.003 | 1.00 | 0.25 |
| PHE97 | H | 1.00 | 0.010 | 1.00 | 0.11 |

3.97.4 Detailed Probabilities of PHE97CD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE97 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F97HA | 1.00 |
| F97HB2 | 1.00 |
| F97HB3 | 1.00 |
| F97HD1 | 1.00 |
| F97HE1 | 1.00 |
| F97HE2 | 1.00 |
| F97HZ | 1.00 |
| F97H | 0.99 |
| F97HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE97 | HA | 1.00 | 0.002 | 1.00 | 0.58 |
| PHE97 | HB2 | 1.00 | 0.006 | 1.00 | 0.12 |
| PHE97 | HB3 | 1.00 | 0.000 | 1.00 | 0.76 |
| PHE97 | HD1 | 1.00 | 0.003 | 1.00 | 4.75 |
| PHE97 | HD2 | 1.00 | 0.003 | 1.00 | 4.75 |
| PHE97 | HE1 | 1.00 | 0.001 | 1.00 | 0.58 |
| PHE97 | HE2 | 1.00 | 0.001 | 1.00 | 0.58 |
| PHE97 | HZ | 1.00 | 0.003 | 1.00 | 0.25 |
| PHE97 | H | 0.99 | 0.010 | 1.00 | 0.11 |

3.97.5 Detailed Probabilities of PHE97CE1:

Overall probability: 0.400

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE97 | 0.40 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F97HD1 | 1.00 |
| F97HD2 | 1.00 |
| F97HE2 | 1.00 |
| F97HZ | 1.00 |
| F97HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE97 | HD1 | 1.00 | 0.003 | 1.00 | 0.56 |
| PHE97 | HD2 | 1.00 | 0.003 | 1.00 | 0.56 |
| PHE97 | HE1 | 1.00 | 0.359 | 0.00 | 0.00 |
| PHE97 | HE2 | 1.00 | 0.359 | 0.00 | 0.00 |
| PHE97 | HZ | 1.00 | 0.387 | 0.00 | 0.00 |

3.97.6 Detailed Probabilities of PHE97CE2:

Overall probability: 0.286

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE97 | 0.29 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F97HB2 | 1.00 |
| F97HB3 | 1.00 |
| F97HD1 | 1.00 |
| F97HD2 | 1.00 |
| F97HE1 | 1.00 |
| F97HZ | 1.00 |
| F97HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE97 | HB2 | 1.00 | 1.028 | 0.00 | 0.00 |
| PHE97 | HB3 | 1.00 | 1.178 | 0.00 | 0.00 |
| PHE97 | HD1 | 1.00 | 0.003 | 1.00 | 0.56 |
| PHE97 | HD2 | 1.00 | 0.003 | 1.00 | 0.56 |
| PHE97 | HE1 | 1.00 | 0.359 | 0.00 | 0.00 |
| PHE97 | HE2 | 1.00 | 0.359 | 0.00 | 0.00 |
| PHE97 | HZ | 1.00 | 0.387 | 0.00 | 0.00 |

3.97.7 Detailed Probabilities of PHE97CZ:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE97 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F97HD1 | 1.00 |
| F97HD2 | 1.00 |
| F97HE1 | 1.00 |
| F97HE2 | 1.00 |
| F97HZ | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE97 | HD1 | 1.00 | 0.002 | 1.00 | 0.09 |
| PHE97 | HD2 | 1.00 | 0.002 | 1.00 | 0.09 |
| PHE97 | HE1 | 1.00 | 0.001 | 1.00 | 3.47 |
| PHE97 | HE2 | 1.00 | 0.001 | 1.00 | 3.47 |
| PHE97 | HZ | 1.00 | 0.000 | 1.00 | 13.47 |

3.97.8 Detailed Probabilities of PHE97N:

Overall probability: 0.915

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE96 | 0.82 | 1.00 |
| PHE97 | 1.00 | 1.00 |
| ALA98 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F96HB3 | 1.00 |
| F96HB2 | 1.00 |
| F96HA | 1.00 |
| F96H | 1.00 |
| F97HA | 1.00 |
| F97HB2 | 1.00 |
| F97HB3 | 1.00 |
| F97HD1 | 1.00 |
| F97HD2 | 0.99 |
| F97H | 1.00 |
| A98H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE96 | HA | 1.00 | 0.031 | 0.90 | 0.00 |
| PHE96 | HB2 | 1.00 | 0.066 | 0.00 | 0.00 |
| PHE96 | HB3 | 1.00 | 0.007 | 1.00 | -823040.00 |
| PHE96 | H | 1.00 | 0.003 | 1.00 | -876987.00 |
| PHE96 | HD1 | 0.79 | 0.007 | 1.00 | -422400.00 |
| PHE96 | HD2 | 0.70 | 0.007 | 1.00 | -422400.00 |
| PHE97 | HA | 1.00 | 0.004 | 1.00 | -952702.00 |
| PHE97 | HB2 | 1.00 | 0.005 | 1.00 | -1253342.00 |
| PHE97 | HB3 | 1.00 | 0.004 | 1.00 | -839166.00 |
| PHE97 | HD1 | 1.00 | 0.004 | 1.00 | -682945.00 |
| PHE97 | HD2 | 0.99 | 0.004 | 1.00 | -682945.00 |
| PHE97 | H | 1.00 | 0.005 | 1.00 | -9168664.00 |
| ALA98 | H | 1.00 | 0.001 | 1.00 | -1044861.00 |

3.97.9 Detailed Probabilities of PHE97HA:

Overall probability: 0.853

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE96 | 0.80 | 1.00 |
| PHE97 | 1.00 | 1.00 |
| ALA98 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F96HA | 1.00 |
| F97HB2 | 1.00 |
| F97HB3 | 1.00 |
| F97HD1 | 1.00 |
| F97HD2 | 1.00 |
| F97H | 1.00 |
| F97HA | 1.00 |
| A98HA | 1.00 |
| A98H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE96 | HA | 1.00 | 0.034 | 0.60 | 0.00 |
| PHE96 | HB3 | 0.88 | 0.035 | 0.88 | 0.00 |
| PHE96 | H | 0.90 | 0.032 | 0.90 | 0.00 |
| PHE97 | HA | 1.00 | 0.000 | 1.00 | 6.88 |
| PHE97 | HB2 | 1.00 | 0.014 | 1.00 | 0.45 |
| PHE97 | HB3 | 1.00 | 0.013 | 1.00 | 0.62 |
| PHE97 | HD1 | 1.00 | 0.002 | 1.00 | 0.58 |
| PHE97 | HD2 | 1.00 | 0.002 | 1.00 | 0.58 |
| PHE97 | H | 1.00 | 0.004 | 1.00 | -952702.00 |
| ALA98 | HA | 1.00 | 0.010 | 1.00 | 0.15 |
| ALA98 | H | 1.00 | 0.224 | 0.00 | 0.00 |

3.97.10 Detailed Probabilities of PHE97HB2:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE97 | 0.86 | 1.00 |
| ALA98 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F97HA | 1.00 |
| F97HB3 | 1.00 |
| F97HD1 | 1.00 |
| F97HD2 | 1.00 |
| F97HE2 | 1.00 |
| F97H | 1.00 |
| F97HB2 | 1.00 |
| A98H | 1.00 |

NOESY contacts detailed probability

3.97 PHE(97)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE97 | HA | 1.00 | 0.010 | 1.00 | 0.43 |
| PHE97 | HB2 | 1.00 | 0.004 | 1.00 | 2.08 |
| PHE97 | HB3 | 1.00 | 0.001 | 1.00 | 2.38 |
| PHE97 | HD1 | 1.00 | 0.006 | 1.00 | 0.12 |
| PHE97 | HD2 | 1.00 | 0.006 | 1.00 | 0.12 |
| PHE97 | HE2 | 1.00 | 1.028 | 0.00 | 0.00 |
| PHE97 | H | 1.00 | 0.005 | 1.00 | -1253342.00 |
| ALA98 | H | 1.00 | 0.006 | 1.00 | -477023.00 |

3.97.11 Detailed Probabilities of PHE97HB3:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE97 | 0.86 | 1.00 |
| ALA98 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F97HA | 1.00 |
| F97HB2 | 1.00 |
| F97HD1 | 1.00 |
| F97HD2 | 1.00 |
| F97HE2 | 1.00 |
| F97H | 1.00 |
| F97HB3 | 1.00 |
| A98H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE97 | HA | 1.00 | 0.000 | 1.00 | 0.63 |
| PHE97 | HB2 | 1.00 | 0.009 | 1.00 | 2.17 |
| PHE97 | HB3 | 1.00 | 0.020 | 1.00 | 5.26 |
| PHE97 | HD1 | 1.00 | 0.000 | 1.00 | 0.76 |
| PHE97 | HD2 | 1.00 | 0.000 | 1.00 | 0.76 |
| PHE97 | HE2 | 1.00 | 1.178 | 0.00 | 0.00 |
| PHE97 | H | 1.00 | 0.004 | 1.00 | -839166.00 |
| ALA98 | H | 1.00 | 0.005 | 1.00 | -358842.00 |

3.97.12 Detailed Probabilities of PHE97HD1:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE97 | 0.89 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F97HA | 1.00 |
| F97HB2 | 1.00 |
| F97HB3 | 1.00 |
| F97HD2 | 1.00 |
| F97HE1 | 1.00 |
| F97HE2 | 1.00 |
| F97HZ | 1.00 |
| F97H | 1.00 |
| F97HD1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE97 | HA | 1.00 | 0.292 | 0.00 | 0.00 |
| PHE97 | HB2 | 1.00 | 0.005 | 1.00 | 0.33 |
| PHE97 | HB3 | 1.00 | 0.006 | 1.00 | 0.43 |
| PHE97 | HD1 | 1.00 | 0.003 | 1.00 | 4.75 |
| PHE97 | HD2 | 1.00 | 0.003 | 1.00 | 4.75 |
| PHE97 | HE1 | 1.00 | 0.003 | 1.00 | 0.56 |
| PHE97 | HE2 | 1.00 | 0.003 | 1.00 | 0.56 |
| PHE97 | HZ | 1.00 | 0.002 | 1.00 | 0.09 |
| PHE97 | H | 1.00 | 0.004 | 1.00 | -682945.00 |

3.97.13 Detailed Probabilities of PHE97HD2:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE97 | 0.89 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F97HA | 1.00 |
| F97HB2 | 1.00 |
| F97HB3 | 1.00 |
| F97HD1 | 1.00 |
| F97HE1 | 1.00 |
| F97HE2 | 1.00 |
| F97HZ | 1.00 |
| F97H | 0.99 |
| F97HD2 | 1.00 |

NOESY contacts detailed probability

3.97 PHE(97)

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE97 | HA | 1.00 | 0.292 | 0.00 | 0.00 |
| PHE97 | HB2 | 1.00 | 0.005 | 1.00 | 0.33 |
| PHE97 | HB3 | 1.00 | 0.006 | 1.00 | 0.43 |
| PHE97 | HD1 | 1.00 | 0.003 | 1.00 | 4.75 |
| PHE97 | HD2 | 1.00 | 0.003 | 1.00 | 4.75 |
| PHE97 | HE1 | 1.00 | 0.003 | 1.00 | 0.56 |
| PHE97 | HE2 | 1.00 | 0.003 | 1.00 | 0.56 |
| PHE97 | HZ | 1.00 | 0.002 | 1.00 | 0.09 |
| PHE97 | H | 0.99 | 0.004 | 1.00 | -682945.00 |

3.97.14 Detailed Probabilities of PHE97HE1:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE97 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F97HD1 | 1.00 |
| F97HD2 | 1.00 |
| F97HE2 | 1.00 |
| F97HZ | 1.00 |
| F97HE1 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE97 | HD1 | 1.00 | 0.001 | 1.00 | 0.58 |
| PHE97 | HD2 | 1.00 | 0.001 | 1.00 | 0.58 |
| PHE97 | HE1 | 1.00 | 0.359 | 0.00 | 0.00 |
| PHE97 | HE2 | 1.00 | 0.359 | 0.00 | 0.00 |
| PHE97 | HZ | 1.00 | 0.001 | 1.00 | 3.47 |
| PHE97 | HA | 0.74 | 0.009 | 1.00 | 0.12 |
| PHE97 | HB2 | 0.90 | 0.009 | 1.00 | 0.08 |

3.97.15 Detailed Probabilities of PHE97HE2:

Overall probability: 0.572

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE97 | 0.57 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F97HB2 | 1.00 |
| F97HB3 | 1.00 |
| F97HD1 | 1.00 |
| F97HD2 | 1.00 |
| F97HE1 | 1.00 |
| F97HZ | 1.00 |
| F97HE2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE97 | HB2 | 1.00 | 0.009 | 1.00 | 0.08 |
| PHE97 | HB3 | 1.00 | 0.206 | 0.00 | 0.00 |
| PHE97 | HD1 | 1.00 | 0.001 | 1.00 | 0.58 |
| PHE97 | HD2 | 1.00 | 0.001 | 1.00 | 0.58 |
| PHE97 | HE1 | 1.00 | 0.359 | 0.00 | 0.00 |
| PHE97 | HE2 | 1.00 | 0.359 | 0.00 | 0.00 |
| PHE97 | HZ | 1.00 | 0.001 | 1.00 | 3.47 |

3.97.16 Detailed Probabilities of PHE97HZ:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE97 | 0.60 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F97HD1 | 1.00 |
| F97HD2 | 1.00 |
| F97HE1 | 1.00 |
| F97HE2 | 1.00 |
| F97HZ | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE97 | HD1 | 1.00 | 0.003 | 1.00 | 0.25 |
| PHE97 | HD2 | 1.00 | 0.003 | 1.00 | 0.25 |
| PHE97 | HE1 | 1.00 | 0.387 | 0.00 | 0.00 |
| PHE97 | HE2 | 1.00 | 0.387 | 0.00 | 0.00 |
| PHE97 | HZ | 1.00 | 0.000 | 1.00 | 13.47 |

3.97.17 Detailed Probabilities of PHE97H:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE96 | 0.67 | 1.00 |
| PHE97 | 1.00 | 1.00 |
| ALA98 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F96HB3 | 1.00 |
| F96HB2 | 1.00 |
| F96HA | 1.00 |
| F96H | 1.00 |
| F97HA | 1.00 |
| F97HB2 | 1.00 |
| F97HB3 | 1.00 |
| F97HD1 | 1.00 |
| F97HD2 | 0.99 |
| F97H | 1.00 |
| A98H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE96 | HA | 1.00 | 0.387 | 0.00 | 0.00 |
| PHE96 | HB2 | 1.00 | 0.006 | 1.00 | 0.25 |
| PHE96 | HB3 | 1.00 | 0.384 | 0.00 | 0.00 |
| PHE96 | H | 1.00 | 0.016 | 1.00 | -854700.00 |
| PHE96 | HD1 | 0.79 | 0.002 | 1.00 | 0.13 |
| PHE96 | HD2 | 0.70 | 0.002 | 1.00 | 0.13 |
| PHE97 | HA | 1.00 | 0.007 | 1.00 | 0.46 |
| PHE97 | HB2 | 1.00 | 0.007 | 1.00 | 0.45 |
| PHE97 | HB3 | 1.00 | 0.007 | 1.00 | 0.45 |
| PHE97 | HD1 | 1.00 | 0.010 | 1.00 | 0.11 |
| PHE97 | HD2 | 0.99 | 0.010 | 1.00 | 0.11 |
| PHE97 | H | 1.00 | 0.005 | 1.00 | -9168664.00 |
| ALA98 | H | 1.00 | 0.005 | 1.00 | -1274320.00 |
| ALA98 | HA | 0.84 | 0.007 | 1.00 | 0.06 |

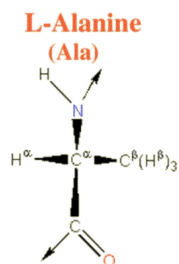
3.98 ALA(98)

Figure 88: Image from the BMRB

Residue probability: 0.824

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-----------|-------------|---------|--------|---------------------|--------------------|
| CA 3.98.1 | 53.463 | 53.289 | 3.425 | 0.857 | 1.000 |
| CB 3.98.2 | 18.168 | 19.355 | 4.103 | 1.000 | 1.000 |
| N 3.98.3 | 121.061 | 123.100 | 4.487 | 0.625 | 1.000 |
| HA 3.98.4 | 4.247 | 4.254 | 0.459 | 0.713 | 1.000 |
| HB 3.98.5 | 1.469 | 1.346 | 0.258 | 1.000 | 1.000 |
| H 3.98.6 | 7.869 | 8.206 | 0.601 | 0.750 | 1.000 |

3.98.1 Detailed Probabilities of ALA98CA:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE97 | 1.00 | 1.00 |
| ALA98 | 1.00 | 1.00 |
| SER99 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F97HA | 1.00 |
| A98H | 1.00 |
| A98HB1 | 1.00 |
| A98HA | 1.00 |
| S99HA | 1.00 |
| S99H | 1.00 |

NOESY contacts detailed probability

3.98 ALA(98)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE97 | HA | 1.00 | 0.010 | 1.00 | 0.15 |
| PHE97 | H | 0.84 | 0.007 | 1.00 | 0.06 |
| ALA98 | HA | 1.00 | 0.002 | 1.00 | 13.33 |
| ALA98 | HB1 | 1.00 | 0.000 | 1.00 | 3.37 |
| ALA98 | H | 1.00 | 0.000 | 1.00 | 0.77 |
| SER99 | HA | 1.00 | 0.104 | 0.00 | 0.00 |
| SER99 | H | 1.00 | 0.001 | 1.00 | 0.24 |

3.98.2 Detailed Probabilities of ALA98CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA98 | 1.00 | 1.00 |
| SER99 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A98HA | 1.00 |
| A98H | 1.00 |
| A98HB2 | 1.00 |
| S99H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA98 | HA | 1.00 | 0.002 | 1.00 | 3.34 |
| ALA98 | HB1 | 1.00 | 0.000 | 1.00 | 64.31 |
| ALA98 | H | 1.00 | 0.001 | 1.00 | 2.36 |
| SER99 | H | 1.00 | 0.002 | 1.00 | 0.57 |
| SER99 | HA | 0.70 | 0.010 | 1.00 | 0.38 |

3.98.3 Detailed Probabilities of ALA98N:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE97 | 0.75 | 1.00 |
| ALA98 | 0.67 | 1.00 |
| SER99 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F97HB3 | 1.00 |
| F97HB2 | 1.00 |
| F97H | 1.00 |
| F97HA | 1.00 |
| A98HA | 1.00 |
| A98HB1 | 1.00 |
| A98H | 1.00 |
| S99H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE97 | HA | 1.00 | 0.224 | 0.00 | 0.00 |
| PHE97 | HB2 | 1.00 | 0.006 | 1.00 | -477023.00 |
| PHE97 | HB3 | 1.00 | 0.005 | 1.00 | -358842.00 |
| PHE97 | H | 1.00 | 0.005 | 1.00 | -1274320.00 |
| ALA98 | HA | 1.00 | 0.002 | 1.00 | -1612471.00 |
| ALA98 | HB1 | 1.00 | 0.001 | 1.00 | -4446864.00 |
| ALA98 | H | 1.00 | 0.103 | 0.00 | 0.00 |
| SER99 | H | 1.00 | 0.341 | 0.00 | 0.00 |

3.98.4 Detailed Probabilities of ALA98HA:

Overall probability: 0.713

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE97 | 0.60 | 1.00 |
| ALA98 | 1.00 | 1.00 |
| SER99 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F97HA | 1.00 |
| A98H | 1.00 |
| A98HB1 | 1.00 |
| A98HA | 1.00 |
| S99HA | 1.00 |
| S99H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE97 | HA | 1.00 | 0.043 | 0.00 | 0.00 |
| PHE97 | HB2 | 0.61 | 0.034 | 0.61 | 0.00 |
| PHE97 | HB3 | 0.78 | 0.032 | 0.80 | 0.00 |
| PHE97 | H | 0.84 | 0.030 | 1.00 | 0.00 |
| ALA98 | HA | 1.00 | 0.002 | 1.00 | 13.33 |
| ALA98 | HB1 | 1.00 | 0.002 | 1.00 | 3.34 |
| ALA98 | H | 1.00 | 0.002 | 1.00 | -1612471.00 |
| SER99 | HA | 1.00 | 0.075 | 0.00 | 0.00 |
| SER99 | H | 1.00 | 0.003 | 1.00 | -649755.00 |

3.98.5 Detailed Probabilities of ALA98HB1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA98 | 1.00 | 1.00 |
| SER99 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A98HA | 1.00 |
| A98H | 1.00 |
| A98HB2 | 1.00 |
| S99H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA98 | HA | 1.00 | 0.000 | 1.00 | 3.37 |
| ALA98 | HB1 | 1.00 | 0.000 | 1.00 | 64.31 |
| ALA98 | H | 1.00 | 0.001 | 1.00 | -4446864.00 |
| SER99 | H | 1.00 | 0.002 | 1.00 | -1884341.00 |
| SER99 | HA | 0.70 | 0.001 | 1.00 | 0.73 |

3.98.6 Detailed Probabilities of ALA98H:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PHE97 | 0.75 | 1.00 |
| ALA98 | 0.67 | 1.00 |
| SER99 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| F97HB3 | 1.00 |
| F97HB2 | 1.00 |
| F97H | 1.00 |
| F97HA | 1.00 |
| A98HA | 1.00 |
| A98HB1 | 1.00 |
| A98H | 1.00 |
| S99H | 1.00 |

NOESY contacts detailed probability

3.98 ALA(98)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PHE97 | HA | 1.00 | 0.002 | 1.00 | 0.17 |
| PHE97 | HB2 | 1.00 | 0.002 | 1.00 | 0.13 |
| PHE97 | HB3 | 1.00 | 0.079 | 0.00 | 0.00 |
| PHE97 | H | 1.00 | 0.001 | 1.00 | -1044861.00 |
| ALA98 | HA | 1.00 | 0.000 | 1.00 | 0.77 |
| ALA98 | HB1 | 1.00 | 0.001 | 1.00 | 2.36 |
| ALA98 | H | 1.00 | 0.103 | 0.00 | 0.00 |
| SER99 | H | 1.00 | 0.000 | 1.00 | -1985388.00 |

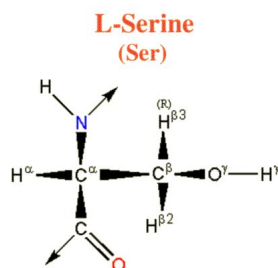
3.99 SER(99)

Figure 89: Image from the BMRB

Residue probability: 0.827

Residue probability confidence: 0.865

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|------------|-------------|---------|--------|---------------------|--------------------|
| C | 175.366 | 174.682 | 1.868 | 0.000 | 0.000 |
| CA 3.99.1 | 60.428 | 58.750 | 3.025 | 0.889 | 0.889 |
| CB 3.99.2 | 64.234 | 63.523 | 4.288 | 0.857 | 0.833 |
| N 3.99.3 | 113.149 | 116.135 | 5.326 | 1.000 | 0.889 |
| HA 3.99.4 | 4.145 | 4.486 | 0.430 | 0.667 | 0.889 |
| HB2 3.99.5 | 3.975 | 3.856 | 0.325 | 0.857 | 0.833 |
| HB3 3.99.6 | 3.808 | 3.825 | 0.343 | 0.633 | 0.833 |
| H 3.99.7 | 7.536 | 8.292 | 0.600 | 0.889 | 0.889 |
| HG | NA | - | - | 0.000 | 0.000 |

3.99.1 Detailed Probabilities of SER99CA:

Overall probability: 0.889

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA98 | 0.50 | 1.00 |
| SER99 | 1.00 | 0.80 |
| GLY100 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| A98HA | 1.00 |
| S99HB2 | 1.00 |
| S99HB3 | 1.00 |
| S99H | 1.00 |
| S99HG | 1.00 |
| S99HA | 1.00 |
| G100HA3 | 1.00 |
| G100HA2 | 1.00 |
| G100H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA98 | HA | 1.00 | 0.075 | 0.00 | 0.00 |
| ALA98 | HB1 | 0.66 | 0.001 | 1.00 | 0.73 |
| SER99 | HA | 1.00 | 0.001 | 1.00 | 14.00 |
| SER99 | HB2 | 1.00 | 0.002 | 1.00 | 1.48 |
| SER99 | HB3 | 1.00 | 0.000 | 1.00 | 1.71 |
| SER99 | H | 1.00 | 0.003 | 1.00 | 0.68 |
| GLY100 | HA2 | 1.00 | 0.010 | 1.00 | 0.17 |
| GLY100 | HA3 | 1.00 | 0.020 | 1.00 | 1.48 |
| GLY100 | H | 1.00 | 0.000 | 1.00 | 0.23 |

3.99.2 Detailed Probabilities of SER99CB:

Overall probability: 0.857

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER99 | 1.00 | 0.80 |
| GLY100 | 0.67 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S99HA | 1.00 |
| S99HB3 | 1.00 |
| S99H | 1.00 |
| S99HG | 1.00 |
| S99HB2 | 1.00 |
| G100H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER99 | HA | 1.00 | 0.005 | 1.00 | 0.74 |
| SER99 | HB2 | 1.00 | 0.000 | 1.00 | 1.60 |
| SER99 | HB3 | 1.00 | 0.001 | 1.00 | 1.56 |
| SER99 | H | 1.00 | 0.001 | 1.00 | 0.36 |
| GLY100 | H | 1.00 | 0.096 | 0.00 | 0.00 |
| GLY100 | HA2 | 0.56 | 0.012 | 1.00 | 0.12 |
| GLY100 | HA3 | 0.53 | 0.022 | 1.00 | 1.60 |

3.99.3 Detailed Probabilities of SER99N:

Overall probability: 1.000

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA98 | 1.00 | 1.00 |
| SER99 | 1.00 | 0.80 |
| GLY100 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A98HB2 | 1.00 |
| A98HA | 1.00 |
| A98H | 1.00 |
| S99HA | 1.00 |
| S99HB2 | 1.00 |
| S99HB3 | 1.00 |
| S99HG | 1.00 |
| S99H | 1.00 |
| G100H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA98 | HA | 1.00 | 0.003 | 1.00 | -649755.00 |
| ALA98 | HB1 | 1.00 | 0.002 | 1.00 | -1884341.00 |
| ALA98 | H | 1.00 | 0.000 | 1.00 | -1985388.00 |
| SER99 | HA | 1.00 | 0.004 | 1.00 | -1290822.00 |
| SER99 | HB2 | 1.00 | 0.001 | 1.00 | -1424217.00 |
| SER99 | HB3 | 1.00 | 0.005 | 1.00 | -830211.00 |
| SER99 | H | 1.00 | 0.000 | 1.00 | -13101264.00 |
| GLY100 | H | 1.00 | 0.002 | 1.00 | -828720.00 |
| GLY100 | HA2 | 0.68 | 0.011 | 1.00 | -189953.00 |
| GLY100 | HA3 | 0.71 | 0.021 | 1.00 | -1424217.00 |

3.99.4 Detailed Probabilities of SER99HA:

Overall probability: 0.667

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA98 | 0.50 | 1.00 |
| SER99 | 1.00 | 0.80 |
| GLY100 | 0.33 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| A98HA | 1.00 |
| S99HB2 | 1.00 |
| S99HB3 | 1.00 |
| S99H | 1.00 |
| S99HG | 1.00 |
| S99HA | 1.00 |
| G100HA3 | 1.00 |
| G100HA2 | 1.00 |
| G100H | 1.00 |

NOESY contacts detailed probability

3.99 SER(99)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA98 | HA | 1.00 | 0.104 | 0.00 | 0.00 |
| ALA98 | HB1 | 0.66 | 0.010 | 1.00 | 0.38 |
| SER99 | HA | 1.00 | 0.001 | 1.00 | 14.00 |
| SER99 | HB2 | 1.00 | 0.005 | 1.00 | 0.74 |
| SER99 | HB3 | 1.00 | 0.003 | 1.00 | 0.91 |
| SER99 | H | 1.00 | 0.004 | 1.00 | -1290822.00 |
| GLY100 | HA2 | 1.00 | 0.102 | 0.00 | 0.00 |
| GLY100 | HA3 | 1.00 | 0.151 | 0.00 | 0.00 |
| GLY100 | H | 1.00 | 0.012 | 1.00 | -258524.00 |

3.99.5 Detailed Probabilities of SER99HB2:

Overall probability: 0.857

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER99 | 0.75 | 0.80 |
| GLY100 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S99HA | 1.00 |
| S99HB3 | 1.00 |
| S99H | 1.00 |
| S99HG | 1.00 |
| S99HB2 | 1.00 |
| G100H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER99 | HA | 1.00 | 0.002 | 1.00 | 1.48 |
| SER99 | HB2 | 1.00 | 0.000 | 1.00 | 1.60 |
| SER99 | HB3 | 1.00 | 0.167 | 0.00 | 0.00 |
| SER99 | H | 1.00 | 0.001 | 1.00 | -1424217.00 |
| GLY100 | H | 1.00 | 0.019 | 1.00 | -1024116.00 |
| GLY100 | HA2 | 0.56 | 0.017 | 1.00 | 3.86 |
| GLY100 | HA3 | 0.53 | 0.019 | 1.00 | 4.77 |

3.99.6 Detailed Probabilities of SER99HB3:

Overall probability: 0.633

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER99 | 0.75 | 0.80 |
| GLY100 | 0.40 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| S99HA | 1.00 |
| S99HB2 | 1.00 |
| S99H | 1.00 |
| S99HG | 1.00 |
| S99HB3 | 1.00 |
| G100H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER99 | HA | 1.00 | 0.000 | 1.00 | 1.71 |
| SER99 | HB2 | 1.00 | 0.001 | 1.00 | 1.56 |
| SER99 | HB3 | 1.00 | 0.334 | 0.00 | 0.00 |
| SER99 | H | 1.00 | 0.005 | 1.00 | -830211.00 |
| GLY100 | H | 1.00 | 0.083 | 0.00 | 0.00 |
| GLY100 | HA3 | 0.62 | 0.032 | 0.80 | 0.00 |

3.99.7 Detailed Probabilities of SER99H:

Overall probability: 0.889

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| ALA98 | 0.67 | 1.00 |
| SER99 | 1.00 | 0.80 |
| GLY100 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|--------|----------------------|
| A98HB2 | 1.00 |
| A98HA | 1.00 |
| A98H | 1.00 |
| S99HA | 1.00 |
| S99HB2 | 1.00 |
| S99HB3 | 1.00 |
| S99HG | 1.00 |
| S99H | 1.00 |
| G100H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| ALA98 | HA | 1.00 | 0.001 | 1.00 | 0.24 |
| ALA98 | HB1 | 1.00 | 0.002 | 1.00 | 0.57 |
| ALA98 | H | 1.00 | 0.341 | 0.00 | 0.00 |
| SER99 | HA | 1.00 | 0.003 | 1.00 | 0.68 |
| SER99 | HB2 | 1.00 | 0.001 | 1.00 | 0.36 |
| SER99 | HB3 | 1.00 | 0.005 | 1.00 | 0.28 |
| SER99 | H | 1.00 | 0.000 | 1.00 | -13101264.00 |
| GLY100 | H | 1.00 | 0.005 | 1.00 | -681352.00 |
| GLY100 | HA2 | 0.68 | 0.007 | 1.00 | 0.07 |

3.100 GLY(100)

Figure 90: Image from the BMRB

Residue probability: 0.873

Residue probability confidence: 0.956

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 173.598 | 173.872 | 2.493 | 0.000 | 0.000 |
| CA 3.100.1 | 45.838 | 45.581 | 4.381 | 0.875 | 1.000 |
| N 3.100.2 | 109.375 | 109.752 | 5.331 | 0.875 | 0.889 |
| HA2 3.100.3 | 3.702 | 3.967 | 0.380 | 0.863 | 1.000 |
| HA3 3.100.4 | 3.997 | 3.897 | 0.390 | 1.000 | 1.000 |
| H 3.100.5 | 7.205 | 8.343 | 0.939 | 0.750 | 0.889 |

3.100.1 Detailed Probabilities of GLY100CA:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER99 | 0.67 | 1.00 |
| GLY100 | 1.00 | 1.00 |
| LEU101 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| S99HA | 1.00 |
| G100HA3 | 1.00 |
| G100H | 1.00 |
| G100HA2 | 1.00 |
| L101HA | 1.00 |
| L101H | 1.00 |

NOESY contacts detailed probability

3.100 GLY(100)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER99 | HA | 1.00 | 0.102 | 0.00 | 0.00 |
| SER99 | HB2 | 0.56 | 0.017 | 1.00 | 3.86 |
| SER99 | H | 0.68 | 0.007 | 1.00 | 0.07 |
| GLY100 | HA2 | 1.00 | 0.002 | 1.00 | 4.20 |
| GLY100 | HA3 | 1.00 | 0.005 | 1.00 | 3.86 |
| GLY100 | H | 1.00 | 0.001 | 1.00 | 0.81 |
| LEU101 | HA | 1.00 | 0.007 | 1.00 | 0.06 |
| LEU101 | H | 1.00 | 0.002 | 1.00 | 0.31 |

3.100.2 Detailed Probabilities of GLY100N:

Overall probability: 0.875

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER99 | 0.75 | 0.80 |
| GLY100 | 1.00 | 1.00 |
| LEU101 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| S99HG | 0.96 |
| S99HB3 | 1.00 |
| S99HB2 | 1.00 |
| S99HA | 1.00 |
| S99H | 1.00 |
| G100HA2 | 1.00 |
| G100HA3 | 1.00 |
| G100H | 1.00 |
| L101H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER99 | HA | 1.00 | 0.012 | 1.00 | -258524.00 |
| SER99 | HB2 | 1.00 | 0.019 | 1.00 | -1024116.00 |
| SER99 | HB3 | 1.00 | 0.083 | 0.00 | 0.00 |
| SER99 | H | 1.00 | 0.005 | 1.00 | -681352.00 |
| GLY100 | HA2 | 1.00 | 0.001 | 1.00 | -1340193.00 |
| GLY100 | HA3 | 1.00 | 0.003 | 1.00 | -1024116.00 |
| GLY100 | H | 1.00 | 0.017 | 1.00 | -13554855.00 |
| LEU101 | H | 1.00 | 0.006 | 1.00 | -788543.00 |

3.100.3 Detailed Probabilities of GLY100HA2:

Overall probability: 0.863

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER99 | 1.00 | 1.00 |
| GLY100 | 0.67 | 1.00 |
| LEU101 | 0.95 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| S99HA | 1.00 |
| G100HA3 | 1.00 |
| G100H | 1.00 |
| G100HA2 | 1.00 |
| L101HA | 1.00 |
| L101H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER99 | HA | 1.00 | 0.010 | 1.00 | 0.17 |
| SER99 | HB2 | 0.56 | 0.012 | 1.00 | 0.12 |
| SER99 | H | 0.68 | 0.011 | 1.00 | -189953.00 |
| GLY100 | HA2 | 1.00 | 0.002 | 1.00 | 4.20 |
| GLY100 | HA3 | 1.00 | 0.138 | 0.00 | 0.00 |
| GLY100 | H | 1.00 | 0.001 | 1.00 | -1340193.00 |
| LEU101 | HA | 1.00 | 0.031 | 0.90 | 0.00 |
| LEU101 | H | 1.00 | 0.000 | 1.00 | -370093.00 |

3.100.4 Detailed Probabilities of GLY100HA3:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER99 | 1.00 | 1.00 |
| GLY100 | 1.00 | 1.00 |
| LEU101 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| S99HA | 1.00 |
| G100HA2 | 1.00 |
| G100H | 1.00 |
| G100HA3 | 1.00 |
| L101HA | 1.00 |
| L101H | 1.00 |

NOESY contacts detailed probability

3.100 GLY(100)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER99 | HA | 1.00 | 0.020 | 1.00 | 1.48 |
| SER99 | HB2 | 0.53 | 0.022 | 1.00 | 1.60 |
| SER99 | H | 0.71 | 0.021 | 1.00 | -1424217.00 |
| GLY100 | HA2 | 1.00 | 0.005 | 1.00 | 3.86 |
| GLY100 | HA3 | 1.00 | 0.003 | 1.00 | 4.77 |
| GLY100 | H | 1.00 | 0.003 | 1.00 | -1024116.00 |
| LEU101 | HA | 1.00 | 0.017 | 1.00 | 0.08 |
| LEU101 | H | 1.00 | 0.009 | 1.00 | -448376.00 |
| LEU101 | HG | 0.53 | 0.007 | 1.00 | 0.11 |

3.100.5 Detailed Probabilities of GLY100H:

Overall probability: 0.750

Overall confidence: 0.889

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| SER99 | 0.50 | 0.80 |
| GLY100 | 1.00 | 1.00 |
| LEU101 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| S99HG | 0.96 |
| S99HB3 | 1.00 |
| S99HB2 | 1.00 |
| S99HA | 1.00 |
| S99H | 1.00 |
| G100HA2 | 1.00 |
| G100HA3 | 1.00 |
| G100H | 1.00 |
| L101H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| SER99 | HA | 1.00 | 0.000 | 1.00 | 0.23 |
| SER99 | HB2 | 1.00 | 0.096 | 0.00 | 0.00 |
| SER99 | HB3 | 1.00 | 0.106 | 0.00 | 0.00 |
| SER99 | H | 1.00 | 0.002 | 1.00 | -828720.00 |
| GLY100 | HA2 | 1.00 | 0.001 | 1.00 | 0.81 |
| GLY100 | HA3 | 1.00 | 0.000 | 1.00 | 0.77 |
| GLY100 | H | 1.00 | 0.017 | 1.00 | -13554855.00 |
| LEU101 | H | 1.00 | 0.001 | 1.00 | -602217.00 |

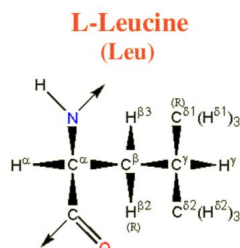
3.101 LEU(101)

Figure 91: Image from the BMRB

Residue probability: 0.672

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|--------------|-------------|---------|--------|---------------------|--------------------|
| C | NA | – | – | 0.000 | 0.000 |
| CA 3.101.1 | 53.452 | 55.735 | 3.802 | 0.960 | 1.000 |
| CB 3.101.2 | 41.284 | 42.389 | 3.750 | 0.444 | 1.000 |
| CG 3.101.3 | 27.245 | 26.892 | 3.086 | 0.143 | 1.000 |
| CD1 3.101.4 | 24.911 | 24.837 | 3.657 | 0.858 | 1.000 |
| CD2 3.101.5 | 22.335 | 24.201 | 3.117 | 0.914 | 1.000 |
| N 3.101.6 | 122.211 | 121.785 | 4.943 | 0.992 | 1.000 |
| HA 3.101.7 | 4.361 | 4.315 | 0.840 | 0.693 | 1.000 |
| HB2 3.101.8 | 1.415 | 1.601 | 0.373 | 0.589 | 1.000 |
| HB3 3.101.9 | 1.297 | 1.508 | 0.398 | 0.667 | 1.000 |
| HG 3.101.10 | 1.463 | 1.510 | 0.340 | 0.500 | 1.000 |
| HD1 3.101.11 | 0.858 | 0.739 | 0.294 | 0.571 | 1.000 |
| HD2 3.101.12 | 0.887 | 0.727 | 0.421 | 0.571 | 1.000 |
| H 3.101.13 | 7.308 | 8.237 | 0.647 | 0.835 | 1.000 |

3.101.1 Detailed Probabilities of LEU101CA:

Overall probability: 0.960

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLY100 | 0.95 | 1.00 |
| LEU101 | 0.93 | 1.00 |
| PRO102 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| G100HA2 | 1.00 |
| G100HA3 | 1.00 |
| L101HB2 | 1.00 |
| L101HB3 | 1.00 |
| L101HG | 1.00 |
| L101HD11 | 0.99 |
| L101HD21 | 0.99 |
| L101H | 1.00 |
| L101HA | 1.00 |
| P102HD2 | 1.00 |
| P102HD3 | 1.00 |
| P102HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLY100 | HA2 | 1.00 | 0.031 | 0.90 | 0.00 |
| GLY100 | HA3 | 1.00 | 0.017 | 1.00 | 0.08 |
| LEU101 | HA | 1.00 | 0.002 | 1.00 | 6.64 |
| LEU101 | HB2 | 1.00 | 0.013 | 1.00 | 0.88 |
| LEU101 | HB3 | 1.00 | 0.004 | 1.00 | 0.45 |
| LEU101 | HG | 1.00 | 0.035 | 0.50 | 0.00 |
| LEU101 | HD11 | 0.99 | 0.025 | 1.00 | 2.17 |
| LEU101 | HD21 | 0.99 | 0.004 | 1.00 | 2.17 |
| LEU101 | H | 1.00 | 0.002 | 1.00 | 0.43 |
| PRO102 | HA | 1.00 | 0.021 | 1.00 | 0.10 |
| PRO102 | HD2 | 1.00 | 0.000 | 1.00 | 1.96 |
| PRO102 | HD3 | 1.00 | 0.007 | 1.00 | 1.41 |
| PRO102 | HB3 | 0.77 | 0.003 | 1.00 | 0.15 |
| PRO102 | HG2 | 0.91 | 0.002 | 1.00 | 0.42 |
| PRO102 | HG3 | 0.90 | 0.001 | 1.00 | 0.42 |

3.101.2 Detailed Probabilities of LEU101CB:

Overall probability: 0.444

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU101 | 0.29 | 1.00 |
| PRO102 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L101HA | 1.00 |
| L101HB2 | 1.00 |
| L101HG | 1.00 |
| L101HD11 | 1.00 |
| L101HD21 | 1.00 |
| L101H | 1.00 |
| L101HB3 | 1.00 |
| P102HD2 | 1.00 |
| P102HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU101 | HA | 1.00 | 0.003 | 1.00 | 0.29 |
| LEU101 | HB2 | 1.00 | 2.177 | 0.00 | 0.00 |
| LEU101 | HB3 | 1.00 | 2.295 | 0.00 | 0.00 |
| LEU101 | HG | 1.00 | 2.129 | 0.00 | 0.00 |
| LEU101 | HD11 | 1.00 | 2.734 | 0.00 | 0.00 |
| LEU101 | HD21 | 1.00 | 2.705 | 0.00 | 0.00 |
| LEU101 | H | 1.00 | 0.003 | 1.00 | 0.43 |
| PRO102 | HD2 | 1.00 | 0.001 | 1.00 | 0.16 |
| PRO102 | HD3 | 1.00 | 0.008 | 1.00 | 0.25 |

3.101.3 Detailed Probabilities of LEU101CG:

Overall probability: 0.143

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU101 | 0.14 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L101HA | 1.00 |
| L101HB2 | 1.00 |
| L101HB3 | 1.00 |
| L101HD11 | 1.00 |
| L101HD21 | 1.00 |
| L101H | 1.00 |
| L101HG | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU101 | HA | 1.00 | 0.109 | 0.00 | 0.00 |
| LEU101 | HB2 | 1.00 | 0.124 | 0.00 | 0.00 |
| LEU101 | HB3 | 1.00 | 0.006 | 1.00 | 1.51 |
| LEU101 | HG | 1.00 | 0.172 | 0.00 | 0.00 |
| LEU101 | HD11 | 1.00 | 0.308 | 0.00 | 0.00 |
| LEU101 | HD21 | 1.00 | 0.279 | 0.00 | 0.00 |
| LEU101 | H | 1.00 | 0.093 | 0.00 | 0.00 |

3.101.4 Detailed Probabilities of LEU101CD1:

Overall probability: 0.858

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU101 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L101HA | 0.99 |
| L101HB2 | 1.00 |
| L101HB3 | 1.00 |
| L101HG | 1.00 |
| L101HD12 | 1.00 |
| L101HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU101 | HA | 0.99 | 0.052 | 0.01 | 0.00 |
| LEU101 | HB2 | 1.00 | 0.029 | 1.00 | 3.10 |
| LEU101 | HB3 | 1.00 | 0.002 | 1.00 | 2.06 |
| LEU101 | HG | 1.00 | 0.019 | 1.00 | 3.10 |
| LEU101 | HD11 | 1.00 | 0.006 | 1.00 | 205.58 |
| LEU101 | HD21 | 1.00 | 0.023 | 1.00 | 205.58 |
| LEU101 | H | 0.86 | 0.004 | 1.00 | 0.49 |

3.101.5 Detailed Probabilities of LEU101CD2:

Overall probability: 0.914

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU101 | 0.91 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L101HA | 0.99 |
| L101HB2 | 1.00 |
| L101HB3 | 1.00 |
| L101HG | 1.00 |
| L101HD11 | 1.00 |
| L101HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU101 | HA | 0.99 | 0.001 | 1.00 | 3.21 |
| LEU101 | HB2 | 1.00 | 0.036 | 0.40 | 0.00 |
| LEU101 | HB3 | 1.00 | 0.006 | 1.00 | 0.69 |
| LEU101 | HG | 1.00 | 0.012 | 1.00 | 3.29 |
| LEU101 | HD11 | 1.00 | 0.028 | 1.00 | 136.50 |
| LEU101 | HD21 | 1.00 | 0.001 | 1.00 | 136.50 |
| LEU101 | H | 0.85 | 0.008 | 1.00 | 0.56 |

3.101.6 Detailed Probabilities of LEU101N:

Overall probability: 0.992

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLY100 | 1.00 | 1.00 |
| LEU101 | 0.99 | 1.00 |
| PRO102 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| G100HA3 | 1.00 |
| G100HA2 | 1.00 |
| G100H | 1.00 |
| L101HA | 1.00 |
| L101HB2 | 1.00 |
| L101HB3 | 1.00 |
| L101HG | 1.00 |
| L101H | 1.00 |
| P102HD2 | 0.99 |
| P102HD3 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLY100 | HA2 | 1.00 | 0.000 | 1.00 | -370093.00 |
| GLY100 | HA3 | 1.00 | 0.009 | 1.00 | -448376.00 |
| GLY100 | H | 1.00 | 0.001 | 1.00 | -602217.00 |
| LEU101 | HA | 1.00 | 0.001 | 1.00 | -884886.00 |
| LEU101 | HB2 | 1.00 | 0.031 | 0.90 | 0.00 |
| LEU101 | HB3 | 1.00 | 0.009 | 1.00 | -1386012.00 |
| LEU101 | HG | 1.00 | 0.017 | 1.00 | -1889980.00 |
| LEU101 | H | 1.00 | 0.002 | 1.00 | -10322191.00 |
| LEU101 | HD11 | 0.88 | 0.011 | 1.00 | -1157950.00 |
| LEU101 | HD21 | 0.87 | 0.018 | 1.00 | -1157950.00 |
| PRO102 | HD2 | 0.99 | 0.003 | 1.00 | -401537.00 |
| PRO102 | HD3 | 0.99 | 0.006 | 1.00 | -214013.00 |

3.101.7 Detailed Probabilities of LEU101HA:

Overall probability: 0.693

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLY100 | 0.50 | 1.00 |
| LEU101 | 0.72 | 1.00 |
| PRO102 | 0.75 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| G100HA2 | 1.00 |
| G100HA3 | 1.00 |
| L101HB2 | 1.00 |
| L101HB3 | 1.00 |
| L101HG | 1.00 |
| L101HD11 | 0.99 |
| L101HD21 | 0.99 |
| L101H | 1.00 |
| L101HA | 1.00 |
| P102HD2 | 1.00 |
| P102HD3 | 1.00 |
| P102HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLY100 | HA2 | 1.00 | 0.007 | 1.00 | 0.06 |
| GLY100 | HA3 | 1.00 | 0.367 | 0.00 | 0.00 |
| LEU101 | HA | 1.00 | 0.002 | 1.00 | 6.64 |
| LEU101 | HB2 | 1.00 | 0.000 | 1.00 | 0.34 |
| LEU101 | HB3 | 1.00 | 0.003 | 1.00 | 0.29 |
| LEU101 | HG | 1.00 | 0.109 | 0.00 | 0.00 |
| LEU101 | HD11 | 0.99 | 0.052 | 0.01 | 0.00 |
| LEU101 | HD21 | 0.99 | 0.001 | 1.00 | 3.21 |
| LEU101 | H | 1.00 | 0.001 | 1.00 | -884886.00 |
| PRO102 | HA | 1.00 | 0.307 | 0.00 | 0.00 |
| PRO102 | HD2 | 1.00 | 0.001 | 1.00 | 1.81 |
| PRO102 | HD3 | 1.00 | 0.000 | 1.00 | 1.57 |
| PRO102 | HB3 | 0.77 | 0.023 | 1.00 | 1.48 |

3.101.8 Detailed Probabilities of LEU101HB2:

Overall probability: 0.589

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU101 | 0.47 | 1.00 |
| PRO102 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L101HA | 1.00 |
| L101HB3 | 1.00 |
| L101HG | 1.00 |
| L101HD11 | 1.00 |
| L101HD21 | 1.00 |
| L101H | 1.00 |
| L101HB2 | 1.00 |
| P102HD3 | 1.00 |
| P102HD2 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU101 | HA | 1.00 | 0.013 | 1.00 | 0.88 |
| LEU101 | HB2 | 1.00 | 0.873 | 0.00 | 0.00 |
| LEU101 | HB3 | 1.00 | 2.177 | 0.00 | 0.00 |
| LEU101 | HG | 1.00 | 0.124 | 0.00 | 0.00 |
| LEU101 | HD11 | 1.00 | 0.029 | 1.00 | 3.10 |
| LEU101 | HD21 | 1.00 | 0.036 | 0.40 | 0.00 |
| LEU101 | H | 1.00 | 0.031 | 0.90 | 0.00 |
| PRO102 | HD2 | 0.99 | 0.001 | 1.00 | 0.52 |
| PRO102 | HD3 | 1.00 | 0.000 | 1.00 | 0.73 |

3.101.9 Detailed Probabilities of LEU101HB3:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU101 | 0.71 | 1.00 |
| PRO102 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L101HA | 1.00 |
| L101HB2 | 1.00 |
| L101HG | 1.00 |
| L101HD11 | 1.00 |
| L101HD21 | 1.00 |
| L101H | 1.00 |
| L101HB3 | 1.00 |
| P102HD2 | 1.00 |
| P102HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU101 | HA | 1.00 | 0.004 | 1.00 | 0.45 |
| LEU101 | HB2 | 1.00 | 0.991 | 0.00 | 0.00 |
| LEU101 | HB3 | 1.00 | 2.295 | 0.00 | 0.00 |
| LEU101 | HG | 1.00 | 0.006 | 1.00 | 1.51 |
| LEU101 | HD11 | 1.00 | 0.002 | 1.00 | 2.06 |
| LEU101 | HD21 | 1.00 | 0.006 | 1.00 | 0.69 |
| LEU101 | H | 1.00 | 0.009 | 1.00 | -1386012.00 |
| PRO102 | HD2 | 1.00 | 0.117 | 0.00 | 0.00 |
| PRO102 | HD3 | 1.00 | 0.016 | 1.00 | 0.36 |

3.101.10 Detailed Probabilities of LEU101HG:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU101 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L101HA | 1.00 |
| L101HB2 | 1.00 |
| L101HB3 | 1.00 |
| L101HD11 | 1.00 |
| L101HD21 | 1.00 |
| L101H | 1.00 |
| L101HG | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU101 | HA | 1.00 | 0.035 | 0.50 | 0.00 |
| LEU101 | HB2 | 1.00 | 0.825 | 0.00 | 0.00 |
| LEU101 | HB3 | 1.00 | 2.129 | 0.00 | 0.00 |
| LEU101 | HG | 1.00 | 0.172 | 0.00 | 0.00 |
| LEU101 | HD11 | 1.00 | 0.019 | 1.00 | 3.10 |
| LEU101 | HD21 | 1.00 | 0.012 | 1.00 | 3.29 |
| LEU101 | H | 1.00 | 0.017 | 1.00 | -1889980.00 |

3.101.11 Detailed Probabilities of LEU101HD11:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU101 | 0.57 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L101HA | 0.99 |
| L101HB2 | 1.00 |
| L101HB3 | 1.00 |
| L101HG | 1.00 |
| L101HD12 | 1.00 |
| L101HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU101 | HA | 0.99 | 0.025 | 1.00 | 2.17 |
| LEU101 | HB2 | 1.00 | 1.430 | 0.00 | 0.00 |
| LEU101 | HB3 | 1.00 | 2.734 | 0.00 | 0.00 |
| LEU101 | HG | 1.00 | 0.308 | 0.00 | 0.00 |
| LEU101 | HD11 | 1.00 | 0.006 | 1.00 | 205.58 |
| LEU101 | HD21 | 1.00 | 0.028 | 1.00 | 136.50 |
| LEU101 | H | 0.86 | 0.011 | 1.00 | -1157950.00 |

3.101.12 Detailed Probabilities of LEU101HD21:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU101 | 0.57 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L101HA | 0.99 |
| L101HB2 | 1.00 |
| L101HB3 | 1.00 |
| L101HG | 1.00 |
| L101HD11 | 1.00 |
| L101HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU101 | HA | 0.99 | 0.004 | 1.00 | 2.17 |
| LEU101 | HB2 | 1.00 | 1.401 | 0.00 | 0.00 |
| LEU101 | HB3 | 1.00 | 2.705 | 0.00 | 0.00 |
| LEU101 | HG | 1.00 | 0.279 | 0.00 | 0.00 |
| LEU101 | HD11 | 1.00 | 0.023 | 1.00 | 205.58 |
| LEU101 | HD21 | 1.00 | 0.001 | 1.00 | 136.50 |
| LEU101 | H | 0.85 | 0.018 | 1.00 | -1157950.00 |

3.101.13 Detailed Probabilities of LEU101H:

Overall probability: 0.835

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLY100 | 1.00 | 1.00 |
| LEU101 | 0.86 | 1.00 |
| PRO102 | 0.51 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| G100HA3 | 1.00 |
| G100HA2 | 1.00 |
| G100H | 1.00 |
| L101HA | 1.00 |
| L101HB2 | 1.00 |
| L101HB3 | 1.00 |
| L101HG | 1.00 |
| L101H | 1.00 |
| P102HD2 | 0.99 |
| P102HD3 | 0.99 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLY100 | HA2 | 1.00 | 0.002 | 1.00 | 0.31 |
| GLY100 | HA3 | 1.00 | 0.000 | 1.00 | 0.30 |
| GLY100 | H | 1.00 | 0.006 | 1.00 | -788543.00 |
| LEU101 | HA | 1.00 | 0.002 | 1.00 | 0.43 |
| LEU101 | HB2 | 1.00 | 0.003 | 1.00 | 0.33 |
| LEU101 | HB3 | 1.00 | 0.003 | 1.00 | 0.43 |
| LEU101 | HG | 1.00 | 0.093 | 0.00 | 0.00 |
| LEU101 | H | 1.00 | 0.002 | 1.00 | -10322191.00 |
| LEU101 | HD11 | 0.88 | 0.004 | 1.00 | 0.49 |
| LEU101 | HD21 | 0.87 | 0.008 | 1.00 | 0.56 |
| PRO102 | HD2 | 0.99 | 0.497 | 0.01 | 0.00 |
| PRO102 | HD3 | 0.99 | 0.002 | 1.00 | 0.12 |

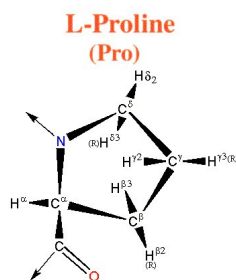
3.102 PRO(102)

Figure 92: Image from the BMRB

Residue probability: 0.675

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|--------------|-------------|---------|--------|---------------------|--------------------|
| C | 176.251 | 175.173 | 13.901 | 0.000 | 0.000 |
| CA 3.102.1 | 61.901 | 62.931 | 15.301 | 0.100 | 1.000 |
| CB 3.102.2 | 31.754 | 33.632 | 13.629 | 1.000 | 1.000 |
| CG 3.102.3 | 27.140 | 28.412 | 13.801 | 0.643 | 1.000 |
| CD 3.102.4 | 50.118 | 49.797 | 3.175 | 0.847 | 1.000 |
| N | NA | – | – | 0.000 | 0.000 |
| HA 3.102.5 | 4.508 | 4.332 | 0.427 | 0.818 | 1.000 |
| HB2 3.102.6 | 1.883 | 2.099 | 0.501 | 0.335 | 1.000 |
| HB3 3.102.7 | 2.325 | 2.052 | 0.596 | 0.625 | 1.000 |
| HG2 3.102.8 | 2.051 | 1.927 | 0.364 | 0.657 | 1.000 |
| HG3 3.102.9 | 2.050 | 1.907 | 0.417 | 0.629 | 1.000 |
| HD2 3.102.10 | 3.798 | 3.640 | 0.682 | 0.929 | 1.000 |
| HD3 3.102.11 | 3.584 | 3.558 | 0.522 | 0.846 | 1.000 |

3.102.1 Detailed Probabilities of PRO102CA:

Overall probability: 0.100

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU101 | 0.00 | 1.00 |
| PRO102 | 0.14 | 1.00 |
| LEU103 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L101HA | 1.00 |
| P102HB2 | 1.00 |
| P102HB3 | 1.00 |
| P102HG2 | 1.00 |
| P102HG3 | 1.00 |
| P102HD2 | 1.00 |
| P102HD3 | 1.00 |
| P102HA | 1.00 |
| L103H | 1.00 |
| L103HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU101 | HA | 1.00 | 0.307 | 0.00 | 0.00 |
| PRO102 | HA | 1.00 | 0.160 | 0.00 | 0.00 |
| PRO102 | HB2 | 1.00 | 0.081 | 0.00 | 0.00 |
| PRO102 | HB3 | 1.00 | 0.099 | 0.00 | 0.00 |
| PRO102 | HG2 | 1.00 | 0.175 | 0.00 | 0.00 |
| PRO102 | HG3 | 1.00 | 0.176 | 0.00 | 0.00 |
| PRO102 | HD2 | 1.00 | 0.008 | 1.00 | 0.06 |
| PRO102 | HD3 | 1.00 | 0.042 | 0.00 | 0.00 |
| LEU103 | HA | 1.00 | 0.046 | 0.00 | 0.00 |
| LEU103 | H | 1.00 | 0.195 | 0.00 | 0.00 |

3.102.2 Detailed Probabilities of PRO102CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO102 | 1.00 | 1.00 |
| LEU103 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P102HA | 1.00 |
| P102HB2 | 1.00 |
| P102HG2 | 1.00 |
| P102HG3 | 1.00 |
| P102HD2 | 1.00 |
| P102HD3 | 1.00 |
| P102HB3 | 1.00 |
| L103H | 1.00 |

NOESY contacts detailed probability

3.102 PRO(102)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO102 | HA | 1.00 | 0.002 | 1.00 | 2.27 |
| PRO102 | HB2 | 1.00 | 0.003 | 1.00 | 6.76 |
| PRO102 | HB3 | 1.00 | 0.009 | 1.00 | 21.15 |
| PRO102 | HG2 | 1.00 | 0.013 | 1.00 | 2.26 |
| PRO102 | HG3 | 1.00 | 0.014 | 1.00 | 2.26 |
| PRO102 | HD2 | 1.00 | 0.009 | 1.00 | 0.62 |
| PRO102 | HD3 | 1.00 | 0.012 | 1.00 | 0.52 |
| LEU103 | H | 1.00 | 0.001 | 1.00 | 0.50 |

3.102.3 Detailed Probabilities of PRO102CG:

Overall probability: 0.643

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO102 | 0.64 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P102HA | 1.00 |
| P102HB2 | 1.00 |
| P102HB3 | 1.00 |
| P102HG3 | 1.00 |
| P102HD2 | 1.00 |
| P102HD3 | 1.00 |
| P102HG2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO102 | HA | 1.00 | 0.003 | 1.00 | 0.51 |
| PRO102 | HB2 | 1.00 | 0.125 | 0.00 | 0.00 |
| PRO102 | HB3 | 1.00 | 0.152 | 0.00 | 0.00 |
| PRO102 | HG2 | 1.00 | 0.032 | 0.80 | 0.00 |
| PRO102 | HG3 | 1.00 | 0.033 | 0.70 | 0.00 |
| PRO102 | HD2 | 1.00 | 0.000 | 1.00 | 1.62 |
| PRO102 | HD3 | 1.00 | 0.011 | 1.00 | 1.62 |

3.102.4 Detailed Probabilities of PRO102CD:

Overall probability: 0.847

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU101 | 0.67 | 1.00 |
| PRO102 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L101HB2 | 0.99 |
| L101H | 0.99 |
| L101HB3 | 1.00 |
| L101HA | 1.00 |
| P102HA | 1.00 |
| P102HB2 | 1.00 |
| P102HB3 | 1.00 |
| P102HG2 | 1.00 |
| P102HG3 | 1.00 |
| P102HD3 | 1.00 |
| P102HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU101 | HA | 1.00 | 0.001 | 1.00 | 1.81 |
| LEU101 | HB2 | 0.99 | 0.001 | 1.00 | 0.52 |
| LEU101 | HB3 | 1.00 | 0.117 | 0.00 | 0.00 |
| LEU101 | H | 0.99 | 0.497 | 0.01 | 0.00 |
| LEU101 | HD11 | 0.63 | 0.025 | 1.00 | 0.81 |
| LEU101 | HD21 | 0.76 | 0.004 | 1.00 | 0.81 |
| PRO102 | HA | 1.00 | 0.008 | 1.00 | 0.21 |
| PRO102 | HB2 | 1.00 | 0.003 | 1.00 | 0.25 |
| PRO102 | HB3 | 1.00 | 0.003 | 1.00 | 0.36 |
| PRO102 | HG2 | 1.00 | 0.004 | 1.00 | 1.38 |
| PRO102 | HG3 | 1.00 | 0.005 | 1.00 | 1.38 |
| PRO102 | HD2 | 1.00 | 0.008 | 1.00 | 5.53 |
| PRO102 | HD3 | 1.00 | 0.013 | 1.00 | 4.34 |

3.102.5 Detailed Probabilities of PRO102HA:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU101 | 1.00 | 1.00 |
| PRO102 | 0.71 | 1.00 |
| LEU103 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L101HA | 1.00 |
| P102HB2 | 1.00 |
| P102HB3 | 1.00 |
| P102HG2 | 1.00 |
| P102HG3 | 1.00 |
| P102HD2 | 1.00 |
| P102HD3 | 1.00 |
| P102HA | 1.00 |
| L103H | 1.00 |
| L103HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU101 | HA | 1.00 | 0.021 | 1.00 | 0.10 |
| PRO102 | HA | 1.00 | 0.160 | 0.00 | 0.00 |
| PRO102 | HB2 | 1.00 | 0.008 | 1.00 | 1.18 |
| PRO102 | HB3 | 1.00 | 0.002 | 1.00 | 2.27 |
| PRO102 | HG2 | 1.00 | 0.003 | 1.00 | 0.51 |
| PRO102 | HG3 | 1.00 | 0.003 | 1.00 | 0.51 |
| PRO102 | HD2 | 1.00 | 0.008 | 1.00 | 0.21 |
| PRO102 | HD3 | 1.00 | 0.139 | 0.00 | 0.00 |
| LEU103 | HA | 1.00 | 0.003 | 1.00 | 0.09 |
| LEU103 | H | 1.00 | 0.000 | 1.00 | -4856998.00 |
| LEU103 | HB2 | 0.65 | 0.003 | 1.00 | 0.18 |

3.102.6 Detailed Probabilities of PRO102HB2:

Overall probability: 0.335

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO102 | 0.29 | 1.00 |
| LEU103 | 0.51 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P102HA | 1.00 |
| P102HB3 | 1.00 |
| P102HG2 | 1.00 |
| P102HG3 | 1.00 |
| P102HD2 | 1.00 |
| P102HD3 | 1.00 |
| P102HB2 | 1.00 |
| L103HA | 0.99 |
| L103H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO102 | HA | 1.00 | 0.081 | 0.00 | 0.00 |
| PRO102 | HB2 | 1.00 | 0.443 | 0.00 | 0.00 |
| PRO102 | HB3 | 1.00 | 0.003 | 1.00 | 6.76 |
| PRO102 | HG2 | 1.00 | 0.125 | 0.00 | 0.00 |
| PRO102 | HG3 | 1.00 | 0.125 | 0.00 | 0.00 |
| PRO102 | HD2 | 1.00 | 0.003 | 1.00 | 0.25 |
| PRO102 | HD3 | 1.00 | 0.096 | 0.00 | 0.00 |
| LEU103 | HA | 0.99 | 0.115 | 0.01 | 0.00 |
| LEU103 | H | 1.00 | 0.000 | 1.00 | -713340.00 |

3.102.7 Detailed Probabilities of PRO102HB3:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO102 | 0.57 | 1.00 |
| LEU103 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P102HA | 1.00 |
| P102HB2 | 1.00 |
| P102HG2 | 1.00 |
| P102HG3 | 1.00 |
| P102HD2 | 1.00 |
| P102HD3 | 1.00 |
| P102HB3 | 1.00 |
| L103H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO102 | HA | 1.00 | 0.099 | 0.00 | 0.00 |
| PRO102 | HB2 | 1.00 | 0.001 | 1.00 | 6.08 |
| PRO102 | HB3 | 1.00 | 0.009 | 1.00 | 21.15 |
| PRO102 | HG2 | 1.00 | 0.152 | 0.00 | 0.00 |
| PRO102 | HG3 | 1.00 | 0.152 | 0.00 | 0.00 |
| PRO102 | HD2 | 1.00 | 0.003 | 1.00 | 0.36 |
| PRO102 | HD3 | 1.00 | 0.001 | 1.00 | 0.35 |
| LEU103 | H | 1.00 | 0.008 | 1.00 | -978304.00 |

3.102.8 Detailed Probabilities of PRO102HG2:

Overall probability: 0.657

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO102 | 0.66 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P102HA | 1.00 |
| P102HB2 | 1.00 |
| P102HB3 | 1.00 |
| P102HG3 | 1.00 |
| P102HD2 | 1.00 |
| P102HD3 | 1.00 |
| P102HG2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO102 | HA | 1.00 | 0.175 | 0.00 | 0.00 |
| PRO102 | HB2 | 1.00 | 0.275 | 0.00 | 0.00 |
| PRO102 | HB3 | 1.00 | 0.013 | 1.00 | 2.26 |
| PRO102 | HG2 | 1.00 | 0.032 | 0.80 | 0.00 |
| PRO102 | HG3 | 1.00 | 0.032 | 0.80 | 0.00 |
| PRO102 | HD2 | 1.00 | 0.004 | 1.00 | 1.38 |
| PRO102 | HD3 | 1.00 | 0.001 | 1.00 | 1.38 |

3.102.9 Detailed Probabilities of PRO102HG3:

Overall probability: 0.629

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO102 | 0.63 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P102HA | 1.00 |
| P102HB2 | 1.00 |
| P102HB3 | 1.00 |
| P102HG2 | 1.00 |
| P102HD2 | 1.00 |
| P102HD3 | 1.00 |
| P102HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO102 | HA | 1.00 | 0.176 | 0.00 | 0.00 |
| PRO102 | HB2 | 1.00 | 0.276 | 0.00 | 0.00 |
| PRO102 | HB3 | 1.00 | 0.014 | 1.00 | 2.26 |
| PRO102 | HG2 | 1.00 | 0.033 | 0.70 | 0.00 |
| PRO102 | HG3 | 1.00 | 0.033 | 0.70 | 0.00 |
| PRO102 | HD2 | 1.00 | 0.005 | 1.00 | 1.38 |
| PRO102 | HD3 | 1.00 | 0.002 | 1.00 | 1.38 |

3.102.10 Detailed Probabilities of PRO102HD2:

Overall probability: 0.929

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU101 | 1.00 | 1.00 |
| PRO102 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L101HB2 | 0.99 |
| L101H | 0.99 |
| L101HB3 | 1.00 |
| L101HA | 1.00 |
| P102HA | 1.00 |
| P102HB2 | 1.00 |
| P102HB3 | 1.00 |
| P102HG2 | 1.00 |
| P102HG3 | 1.00 |
| P102HD3 | 1.00 |
| P102HD2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU101 | HA | 1.00 | 0.000 | 1.00 | 1.96 |
| LEU101 | HB2 | 0.99 | 0.000 | 1.00 | 0.24 |
| LEU101 | HB3 | 1.00 | 0.001 | 1.00 | 0.16 |
| LEU101 | H | 0.99 | 0.003 | 1.00 | -401537.00 |
| LEU101 | HG | 0.94 | 0.005 | 1.00 | 1.03 |
| LEU101 | HD11 | 0.63 | 0.008 | 1.00 | 0.48 |
| LEU101 | HD21 | 0.76 | 0.001 | 1.00 | 1.40 |
| PRO102 | HA | 1.00 | 0.008 | 1.00 | 0.06 |
| PRO102 | HB2 | 1.00 | 0.245 | 0.00 | 0.00 |
| PRO102 | HB3 | 1.00 | 0.009 | 1.00 | 0.62 |
| PRO102 | HG2 | 1.00 | 0.000 | 1.00 | 1.62 |
| PRO102 | HG3 | 1.00 | 0.000 | 1.00 | 1.62 |
| PRO102 | HD2 | 1.00 | 0.008 | 1.00 | 5.53 |
| PRO102 | HD3 | 1.00 | 0.017 | 1.00 | 4.51 |

3.102.11 Detailed Probabilities of PRO102HD3:

Overall probability: 0.846

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU101 | 1.00 | 1.00 |
| PRO102 | 0.71 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| L101HB3 | 1.00 |
| L101H | 0.99 |
| L101HB2 | 1.00 |
| L101HA | 1.00 |
| P102HA | 1.00 |
| P102HB2 | 1.00 |
| P102HB3 | 1.00 |
| P102HG2 | 1.00 |
| P102HG3 | 1.00 |
| P102HD2 | 1.00 |
| P102HD3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU101 | HA | 1.00 | 0.007 | 1.00 | 1.41 |
| LEU101 | HB2 | 1.00 | 0.008 | 1.00 | 0.35 |
| LEU101 | HB3 | 1.00 | 0.008 | 1.00 | 0.25 |
| LEU101 | H | 0.99 | 0.006 | 1.00 | -214013.00 |
| LEU101 | HG | 0.83 | 0.009 | 1.00 | 0.29 |
| LEU101 | HD21 | 0.59 | 0.004 | 1.00 | 1.32 |
| PRO102 | HA | 1.00 | 0.042 | 0.00 | 0.00 |
| PRO102 | HB2 | 1.00 | 0.414 | 0.00 | 0.00 |
| PRO102 | HB3 | 1.00 | 0.012 | 1.00 | 0.52 |
| PRO102 | HG2 | 1.00 | 0.011 | 1.00 | 1.62 |
| PRO102 | HG3 | 1.00 | 0.011 | 1.00 | 1.62 |
| PRO102 | HD2 | 1.00 | 0.013 | 1.00 | 4.34 |
| PRO102 | HD3 | 1.00 | 0.000 | 1.00 | 5.59 |

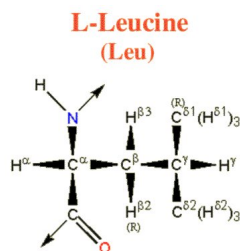
3.103 LEU(103)

Figure 93: Image from the BMRB

Residue probability: 0.839

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|--------------|-------------|---------|--------|---------------------|--------------------|
| C | 177.031 | 177.056 | 1.929 | 0.000 | 0.000 |
| CA 3.103.1 | 57.652 | 55.735 | 3.802 | 0.819 | 1.000 |
| CB 3.103.2 | 42.684 | 42.389 | 3.750 | 1.000 | 1.000 |
| CG 3.103.3 | 27.864 | 26.892 | 3.086 | 1.000 | 1.000 |
| CD1 3.103.4 | 25.452 | 24.837 | 3.657 | 0.287 | 1.000 |
| CD2 3.103.5 | 25.933 | 24.201 | 3.117 | 0.929 | 1.000 |
| N 3.103.6 | 120.233 | 121.785 | 4.943 | 1.000 | 1.000 |
| HA 3.103.7 | 3.989 | 4.315 | 0.840 | 0.638 | 1.000 |
| HB2 3.103.8 | 1.693 | 1.601 | 0.373 | 0.922 | 1.000 |
| HB3 3.103.9 | 1.554 | 1.508 | 0.398 | 0.875 | 1.000 |
| HG 3.103.10 | 1.573 | 1.510 | 0.340 | 0.875 | 1.000 |
| HD1 3.103.11 | 0.548 | 0.739 | 0.294 | 0.786 | 1.000 |
| HD2 3.103.12 | 0.518 | 0.727 | 0.421 | 0.857 | 1.000 |
| H 3.103.13 | 8.358 | 8.237 | 0.647 | 0.923 | 1.000 |

3.103.1 Detailed Probabilities of LEU103CA:

Overall probability: 0.819

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO102 | 0.51 | 1.00 |
| LEU103 | 1.00 | 1.00 |
| VAL104 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| P102HA | 1.00 |
| P102HB2 | 0.99 |
| L103HB2 | 1.00 |
| L103HB3 | 1.00 |
| L103HG | 1.00 |
| L103HD11 | 0.99 |
| L103HD21 | 0.99 |
| L103H | 1.00 |
| L103HA | 1.00 |
| V104H | 1.00 |
| V104HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO102 | HA | 1.00 | 0.003 | 1.00 | 0.09 |
| PRO102 | HB2 | 0.99 | 0.115 | 0.01 | 0.00 |
| LEU103 | HA | 1.00 | 0.011 | 1.00 | 36.36 |
| LEU103 | HB2 | 1.00 | 0.001 | 1.00 | 1.04 |
| LEU103 | HB3 | 1.00 | 0.004 | 1.00 | 1.00 |
| LEU103 | HG | 1.00 | 0.015 | 1.00 | 1.00 |
| LEU103 | HD11 | 0.99 | 0.016 | 1.00 | 1.31 |
| LEU103 | HD21 | 0.99 | 0.014 | 1.00 | 1.31 |
| LEU103 | H | 1.00 | 0.009 | 1.00 | 1.47 |
| VAL104 | HA | 1.00 | 0.407 | 0.00 | 0.00 |
| VAL104 | H | 1.00 | 0.007 | 1.00 | 0.66 |

3.103.2 Detailed Probabilities of LEU103CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU103 | 1.00 | 1.00 |
| VAL104 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L103HA | 1.00 |
| L103HB3 | 1.00 |
| L103HG | 1.00 |
| L103HD11 | 1.00 |
| L103HD21 | 1.00 |
| L103H | 1.00 |
| L103HB2 | 1.00 |
| V104H | 1.00 |

NOESY contacts detailed probability

3.103 LEU(103)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU103 | HA | 1.00 | 0.001 | 1.00 | 0.66 |
| LEU103 | HB2 | 1.00 | 0.003 | 1.00 | 7.45 |
| LEU103 | HB3 | 1.00 | 0.002 | 1.00 | 4.95 |
| LEU103 | HG | 1.00 | 0.017 | 1.00 | 4.95 |
| LEU103 | HD11 | 1.00 | 0.020 | 1.00 | 1.00 |
| LEU103 | HD21 | 1.00 | 0.010 | 1.00 | 1.00 |
| LEU103 | H | 1.00 | 0.000 | 1.00 | 1.21 |
| VAL104 | H | 1.00 | 0.001 | 1.00 | 0.52 |

3.103.3 Detailed Probabilities of LEU103CG:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU103 | 1.00 | 1.00 |
| VAL104 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L103HA | 1.00 |
| L103HB2 | 1.00 |
| L103HB3 | 1.00 |
| L103HD11 | 1.00 |
| L103HD21 | 1.00 |
| L103H | 1.00 |
| L103HG | 1.00 |
| V104H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU103 | HA | 1.00 | 0.000 | 1.00 | 0.37 |
| LEU103 | HB2 | 1.00 | 0.008 | 1.00 | 1.44 |
| LEU103 | HB3 | 1.00 | 0.021 | 1.00 | 15.92 |
| LEU103 | HG | 1.00 | 0.002 | 1.00 | 15.92 |
| LEU103 | HD11 | 1.00 | 0.020 | 1.00 | 1.09 |
| LEU103 | HD21 | 1.00 | 0.010 | 1.00 | 1.09 |
| LEU103 | H | 1.00 | 0.002 | 1.00 | 0.47 |
| VAL104 | H | 0.98 | 0.002 | 1.00 | 0.18 |

3.103.4 Detailed Probabilities of LEU103CD1:

Overall probability: 0.287

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU103 | 0.29 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L103HA | 0.99 |
| L103HB2 | 1.00 |
| L103HB3 | 1.00 |
| L103HG | 1.00 |
| L103HD12 | 1.00 |
| L103HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU103 | HA | 0.99 | 0.110 | 0.01 | 0.00 |
| LEU103 | HB2 | 1.00 | 0.006 | 1.00 | 0.82 |
| LEU103 | HB3 | 1.00 | 0.133 | 0.00 | 0.00 |
| LEU103 | HG | 1.00 | 0.114 | 0.00 | 0.00 |
| LEU103 | HD11 | 1.00 | 0.147 | 0.00 | 0.00 |
| LEU103 | HD21 | 1.00 | 0.117 | 0.00 | 0.00 |
| LEU103 | H | 0.86 | 0.002 | 1.00 | 0.40 |

3.103.5 Detailed Probabilities of LEU103CD2:

Overall probability: 0.929

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU103 | 0.93 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L103HA | 0.99 |
| L103HB2 | 1.00 |
| L103HB3 | 1.00 |
| L103HG | 1.00 |
| L103HD11 | 1.00 |
| L103HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU103 | HA | 0.99 | 0.009 | 1.00 | 0.68 |
| LEU103 | HB2 | 1.00 | 0.006 | 1.00 | 0.82 |
| LEU103 | HB3 | 1.00 | 0.013 | 1.00 | 2.05 |
| LEU103 | HG | 1.00 | 0.006 | 1.00 | 2.05 |
| LEU103 | HD11 | 1.00 | 0.035 | 0.50 | 0.00 |
| LEU103 | HD21 | 1.00 | 0.005 | 1.00 | 110.85 |
| LEU103 | H | 0.85 | 0.001 | 1.00 | 0.36 |

3.103.6 Detailed Probabilities of LEU103N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO102 | 1.00 | 1.00 |
| LEU103 | 1.00 | 1.00 |
| VAL104 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P102HB2 | 1.00 |
| P102HA | 1.00 |
| P102HB3 | 1.00 |
| L103HA | 1.00 |
| L103HB2 | 1.00 |
| L103HB3 | 1.00 |
| L103HG | 1.00 |
| L103H | 1.00 |
| V104H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO102 | HA | 1.00 | 0.000 | 1.00 | -4856998.00 |
| PRO102 | HB2 | 1.00 | 0.000 | 1.00 | -713340.00 |
| PRO102 | HB3 | 1.00 | 0.008 | 1.00 | -978304.00 |
| PRO102 | HG2 | 0.91 | 0.010 | 1.00 | -415404.00 |
| PRO102 | HG3 | 0.74 | 0.011 | 1.00 | -415404.00 |
| PRO102 | HD2 | 0.67 | 0.002 | 1.00 | -104183.00 |
| LEU103 | HA | 1.00 | 0.001 | 1.00 | -1309792.00 |
| LEU103 | HB2 | 1.00 | 0.005 | 1.00 | -2856327.00 |
| LEU103 | HB3 | 1.00 | 0.008 | 1.00 | -2134105.00 |
| LEU103 | HG | 1.00 | 0.011 | 1.00 | -2134105.00 |
| LEU103 | H | 1.00 | 0.001 | 1.00 | -17859134.00 |
| LEU103 | HD11 | 0.88 | 0.018 | 1.00 | -930375.00 |
| LEU103 | HD21 | 0.87 | 0.012 | 1.00 | -930375.00 |
| VAL104 | H | 1.00 | 0.001 | 1.00 | -2261419.00 |
| VAL104 | HA | 0.92 | 0.017 | 1.00 | -81801.00 |

3.103.7 Detailed Probabilities of LEU103HA:

Overall probability: 0.638

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO102 | 0.01 | 1.00 |
| LEU103 | 0.86 | 1.00 |
| VAL104 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| P102HA | 1.00 |
| P102HB2 | 0.99 |
| L103HB2 | 1.00 |
| L103HB3 | 1.00 |
| L103HG | 1.00 |
| L103HD11 | 0.99 |
| L103HD21 | 0.99 |
| L103H | 1.00 |
| L103HA | 1.00 |
| V104H | 1.00 |
| V104HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO102 | HA | 1.00 | 0.046 | 0.00 | 0.00 |
| PRO102 | HB2 | 0.99 | 0.054 | 0.01 | 0.00 |
| LEU103 | HA | 1.00 | 0.011 | 1.00 | 36.36 |
| LEU103 | HB2 | 1.00 | 0.001 | 1.00 | 0.66 |
| LEU103 | HB3 | 1.00 | 0.000 | 1.00 | 0.60 |
| LEU103 | HG | 1.00 | 0.000 | 1.00 | 0.37 |
| LEU103 | HD11 | 0.99 | 0.110 | 0.01 | 0.00 |
| LEU103 | HD21 | 0.99 | 0.009 | 1.00 | 0.68 |
| LEU103 | H | 1.00 | 0.001 | 1.00 | -1309792.00 |
| VAL104 | HA | 1.00 | 0.148 | 0.00 | 0.00 |
| VAL104 | H | 1.00 | 0.001 | 1.00 | -579555.00 |

3.103.8 Detailed Probabilities of LEU103HB2:

Overall probability: 0.922

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU103 | 0.90 | 1.00 |
| VAL104 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L103HA | 1.00 |
| L103HB3 | 1.00 |
| L103HG | 1.00 |
| L103HD11 | 1.00 |
| L103HD21 | 1.00 |
| L103H | 1.00 |
| L103HB2 | 1.00 |
| V104H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU103 | HA | 1.00 | 0.001 | 1.00 | 1.04 |
| LEU103 | HB2 | 1.00 | 0.003 | 1.00 | 7.45 |
| LEU103 | HB3 | 1.00 | 0.037 | 0.30 | 0.00 |
| LEU103 | HG | 1.00 | 0.008 | 1.00 | 1.44 |
| LEU103 | HD11 | 1.00 | 0.006 | 1.00 | 0.82 |
| LEU103 | HD21 | 1.00 | 0.006 | 1.00 | 0.82 |
| LEU103 | H | 1.00 | 0.005 | 1.00 | -2856327.00 |
| VAL104 | H | 1.00 | 0.006 | 1.00 | -1000078.00 |
| VAL104 | HA | 0.59 | 0.010 | 1.00 | 0.15 |

3.103.9 Detailed Probabilities of LEU103HB3:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU103 | 0.86 | 1.00 |
| VAL104 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L103HA | 1.00 |
| L103HB2 | 1.00 |
| L103HG | 1.00 |
| L103HD11 | 1.00 |
| L103HD21 | 1.00 |
| L103H | 1.00 |
| L103HB3 | 1.00 |
| V104H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU103 | HA | 1.00 | 0.004 | 1.00 | 1.00 |
| LEU103 | HB2 | 1.00 | 0.002 | 1.00 | 4.95 |
| LEU103 | HB3 | 1.00 | 0.001 | 1.00 | 7.86 |
| LEU103 | HG | 1.00 | 0.021 | 1.00 | 15.92 |
| LEU103 | HD11 | 1.00 | 0.133 | 0.00 | 0.00 |
| LEU103 | HD21 | 1.00 | 0.013 | 1.00 | 2.05 |
| LEU103 | H | 1.00 | 0.008 | 1.00 | -2134105.00 |
| VAL104 | H | 1.00 | 0.003 | 1.00 | -961740.00 |

3.103.10 Detailed Probabilities of LEU103HG:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU103 | 0.86 | 1.00 |
| VAL104 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L103HA | 1.00 |
| L103HB2 | 1.00 |
| L103HB3 | 1.00 |
| L103HD11 | 1.00 |
| L103HD21 | 1.00 |
| L103H | 1.00 |
| L103HG | 1.00 |
| V104H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU103 | HA | 1.00 | 0.015 | 1.00 | 1.00 |
| LEU103 | HB2 | 1.00 | 0.017 | 1.00 | 4.95 |
| LEU103 | HB3 | 1.00 | 0.020 | 1.00 | 7.86 |
| LEU103 | HG | 1.00 | 0.002 | 1.00 | 15.92 |
| LEU103 | HD11 | 1.00 | 0.114 | 0.00 | 0.00 |
| LEU103 | HD21 | 1.00 | 0.006 | 1.00 | 2.05 |
| LEU103 | H | 1.00 | 0.011 | 1.00 | -2134105.00 |
| VAL104 | H | 0.98 | 0.016 | 1.00 | -961740.00 |

3.103.11 Detailed Probabilities of LEU103HD11:

Overall probability: 0.786

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU103 | 0.79 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L103HA | 0.99 |
| L103HB2 | 1.00 |
| L103HB3 | 1.00 |
| L103HG | 1.00 |
| L103HD12 | 1.00 |
| L103HD21 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU103 | HA | 0.99 | 0.016 | 1.00 | 1.31 |
| LEU103 | HB2 | 1.00 | 0.020 | 1.00 | 1.00 |
| LEU103 | HB3 | 1.00 | 0.025 | 1.00 | 0.97 |
| LEU103 | HG | 1.00 | 0.020 | 1.00 | 1.09 |
| LEU103 | HD11 | 1.00 | 0.147 | 0.00 | 0.00 |
| LEU103 | HD21 | 1.00 | 0.035 | 0.50 | 0.00 |
| LEU103 | H | 0.86 | 0.018 | 1.00 | -930375.00 |

3.103.12 Detailed Probabilities of LEU103HD21:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU103 | 0.86 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L103HA | 0.99 |
| L103HB2 | 1.00 |
| L103HB3 | 1.00 |
| L103HG | 1.00 |
| L103HD11 | 1.00 |
| L103HD22 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU103 | HA | 0.99 | 0.014 | 1.00 | 1.31 |
| LEU103 | HB2 | 1.00 | 0.010 | 1.00 | 1.00 |
| LEU103 | HB3 | 1.00 | 0.005 | 1.00 | 0.97 |
| LEU103 | HG | 1.00 | 0.010 | 1.00 | 1.09 |
| LEU103 | HD11 | 1.00 | 0.117 | 0.00 | 0.00 |
| LEU103 | HD21 | 1.00 | 0.005 | 1.00 | 110.85 |
| LEU103 | H | 0.85 | 0.012 | 1.00 | -930375.00 |

3.103.13 Detailed Probabilities of LEU103H:

Overall probability: 0.923

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| PRO102 | 0.80 | 1.00 |
| LEU103 | 1.00 | 1.00 |
| VAL104 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| P102HB2 | 1.00 |
| P102HA | 1.00 |
| P102HB3 | 1.00 |
| L103HA | 1.00 |
| L103HB2 | 1.00 |
| L103HB3 | 1.00 |
| L103HG | 1.00 |
| L103H | 1.00 |
| V104H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| PRO102 | HA | 1.00 | 0.195 | 0.00 | 0.00 |
| PRO102 | HB2 | 1.00 | 0.005 | 1.00 | 0.42 |
| PRO102 | HB3 | 1.00 | 0.001 | 1.00 | 0.50 |
| PRO102 | HG2 | 0.91 | 0.000 | 1.00 | 0.17 |
| PRO102 | HG3 | 0.74 | 0.000 | 1.00 | 0.17 |
| LEU103 | HA | 1.00 | 0.009 | 1.00 | 1.47 |
| LEU103 | HB2 | 1.00 | 0.000 | 1.00 | 1.21 |
| LEU103 | HB3 | 1.00 | 0.000 | 1.00 | 0.75 |
| LEU103 | HG | 1.00 | 0.002 | 1.00 | 0.47 |
| LEU103 | H | 1.00 | 0.001 | 1.00 | -17859134.00 |
| LEU103 | HD11 | 0.88 | 0.002 | 1.00 | 0.40 |
| LEU103 | HD21 | 0.87 | 0.001 | 1.00 | 0.36 |
| VAL104 | H | 1.00 | 0.001 | 1.00 | -1951678.00 |

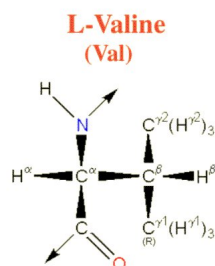
3.104 VAL(104)

Figure 94: Image from the BMRB

Residue probability: 0.779

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 175.132 | 175.682 | 2.367 | 0.000 | 0.000 |
| CA 3.104.1 | 60.271 | 62.613 | 4.828 | 0.556 | 1.000 |
| CB 3.104.2 | 35.104 | 32.918 | 4.591 | 1.000 | 1.000 |
| CG1 3.104.3 | 21.491 | 21.563 | 2.746 | 0.172 | 1.000 |
| CG2 3.104.4 | 20.796 | 21.368 | 2.801 | 0.940 | 1.000 |
| N 3.104.5 | 113.997 | 121.057 | 5.832 | 1.000 | 1.000 |
| HA 3.104.6 | 4.918 | 4.178 | 0.599 | 0.667 | 1.000 |
| HB 3.104.7 | 2.095 | 1.980 | 0.322 | 1.000 | 1.000 |
| HG1 3.104.8 | 1.032 | 0.816 | 0.264 | 0.814 | 1.000 |
| HG2 3.104.9 | 0.998 | 0.803 | 0.504 | 0.800 | 1.000 |
| H 3.104.10 | 7.758 | 8.311 | 0.669 | 0.846 | 1.000 |

3.104.1 Detailed Probabilities of VAL104CA:

Overall probability: 0.556

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU103 | 0.50 | 1.00 |
| VAL104 | 0.80 | 1.00 |
| THR105 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L103HA | 1.00 |
| V104HG11 | 1.00 |
| V104HG21 | 1.00 |
| V104H | 1.00 |
| V104HB | 1.00 |
| V104HA | 1.00 |
| T105H | 1.00 |
| T105HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU103 | HA | 1.00 | 0.148 | 0.00 | 0.00 |
| LEU103 | HB2 | 0.59 | 0.010 | 1.00 | 0.15 |
| VAL104 | HA | 1.00 | 0.016 | 1.00 | 5.02 |
| VAL104 | HB | 1.00 | 0.015 | 1.00 | 0.39 |
| VAL104 | HG11 | 1.00 | 0.005 | 1.00 | 1.04 |
| VAL104 | HG21 | 1.00 | 0.029 | 1.00 | 1.04 |
| VAL104 | H | 1.00 | 0.062 | 0.00 | 0.00 |
| THR105 | HA | 1.00 | 0.069 | 0.00 | 0.00 |
| THR105 | H | 1.00 | 0.094 | 0.00 | 0.00 |

3.104.2 Detailed Probabilities of VAL104CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL104 | 1.00 | 1.00 |
| THR105 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| V104HA | 1.00 |
| V104HG11 | 1.00 |
| V104HG21 | 1.00 |
| V104H | 1.00 |
| V104HB | 1.00 |
| T105H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL104 | HA | 1.00 | 0.008 | 1.00 | 0.53 |
| VAL104 | HB | 1.00 | 0.003 | 1.00 | 19.45 |
| VAL104 | HG11 | 1.00 | 0.012 | 1.00 | 3.14 |
| VAL104 | HG21 | 1.00 | 0.022 | 1.00 | 3.14 |
| VAL104 | H | 1.00 | 0.001 | 1.00 | 0.96 |
| THR105 | H | 1.00 | 0.001 | 1.00 | 0.34 |
| THR105 | HA | 0.79 | 0.018 | 1.00 | 0.06 |

3.104.3 Detailed Probabilities of VAL104CG1:

Overall probability: 0.172

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL104 | 0.20 | 1.00 |
| THR105 | 0.03 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| V104HA | 1.00 |
| V104HG12 | 1.00 |
| V104HG21 | 1.00 |
| V104H | 1.00 |
| V104HB | 1.00 |
| T105H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL104 | HA | 1.00 | 0.426 | 0.00 | 0.00 |
| VAL104 | HB | 1.00 | 0.009 | 1.00 | 4.79 |
| VAL104 | HG11 | 1.00 | 0.187 | 0.00 | 0.00 |
| VAL104 | HG21 | 1.00 | 0.153 | 0.00 | 0.00 |
| VAL104 | H | 1.00 | 0.281 | 0.00 | 0.00 |
| THR105 | H | 0.97 | 0.110 | 0.03 | 0.00 |

3.104.4 Detailed Probabilities of VAL104CG2:

Overall probability: 0.940

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL104 | 0.94 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| V104HA | 1.00 |
| V104HG11 | 1.00 |
| V104HG22 | 1.00 |
| V104H | 1.00 |
| V104HB | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL104 | HA | 1.00 | 0.008 | 1.00 | 0.83 |
| VAL104 | HB | 1.00 | 0.004 | 1.00 | 2.21 |
| VAL104 | HG11 | 1.00 | 0.033 | 0.70 | 0.00 |
| VAL104 | HG21 | 1.00 | 0.001 | 1.00 | 102.88 |
| VAL104 | H | 1.00 | 0.002 | 1.00 | 0.86 |

3.104.5 Detailed Probabilities of VAL104N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU103 | 1.00 | 1.00 |
| VAL104 | 1.00 | 1.00 |
| THR105 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L103HA | 1.00 |
| L103H | 1.00 |
| L103HB3 | 1.00 |
| L103HG | 0.98 |
| L103HB2 | 1.00 |
| V104HA | 1.00 |
| V104HG11 | 1.00 |
| V104HG21 | 1.00 |
| V104HB | 1.00 |
| V104H | 1.00 |
| T105H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU103 | HA | 1.00 | 0.001 | 1.00 | -579555.00 |
| LEU103 | HB2 | 1.00 | 0.006 | 1.00 | -1000078.00 |
| LEU103 | HB3 | 1.00 | 0.003 | 1.00 | -961740.00 |
| LEU103 | HG | 0.98 | 0.016 | 1.00 | -961740.00 |
| LEU103 | H | 1.00 | 0.001 | 1.00 | -1951678.00 |
| LEU103 | HD11 | 0.55 | 0.018 | 1.00 | -327340.00 |
| LEU103 | HD21 | 0.58 | 0.012 | 1.00 | -327340.00 |
| VAL104 | HA | 1.00 | 0.010 | 1.00 | -746382.00 |
| VAL104 | HB | 1.00 | 0.007 | 1.00 | -1665268.00 |
| VAL104 | HG11 | 1.00 | 0.028 | 1.00 | -1494884.00 |
| VAL104 | HG21 | 1.00 | 0.006 | 1.00 | -1494884.00 |
| VAL104 | H | 1.00 | 0.001 | 1.00 | -21124306.00 |
| THR105 | H | 1.00 | 0.003 | 1.00 | -208312.00 |

3.104.6 Detailed Probabilities of VAL104HA:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU103 | 0.50 | 1.00 |
| VAL104 | 0.80 | 1.00 |
| THR105 | 0.50 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L103HA | 1.00 |
| V104HG11 | 1.00 |
| V104HG21 | 1.00 |
| V104H | 1.00 |
| V104HB | 1.00 |
| V104HA | 1.00 |
| T105H | 1.00 |
| T105HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU103 | HA | 1.00 | 0.407 | 0.00 | 0.00 |
| LEU103 | H | 0.92 | 0.017 | 1.00 | -81801.00 |
| VAL104 | HA | 1.00 | 0.016 | 1.00 | 5.02 |
| VAL104 | HB | 1.00 | 0.008 | 1.00 | 0.53 |
| VAL104 | HG11 | 1.00 | 0.426 | 0.00 | 0.00 |
| VAL104 | HG21 | 1.00 | 0.008 | 1.00 | 0.83 |
| VAL104 | H | 1.00 | 0.010 | 1.00 | -746382.00 |
| THR105 | HA | 1.00 | 0.099 | 0.00 | 0.00 |
| THR105 | H | 1.00 | 0.010 | 1.00 | -2603232.00 |

3.104.7 Detailed Probabilities of VAL104HB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL104 | 1.00 | 1.00 |
| THR105 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| V104HA | 1.00 |
| V104HG11 | 1.00 |
| V104HG21 | 1.00 |
| V104H | 1.00 |
| V104HB | 1.00 |
| T105H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL104 | HA | 1.00 | 0.015 | 1.00 | 0.39 |
| VAL104 | HB | 1.00 | 0.003 | 1.00 | 19.45 |
| VAL104 | HG11 | 1.00 | 0.009 | 1.00 | 4.79 |
| VAL104 | HG21 | 1.00 | 0.004 | 1.00 | 2.21 |
| VAL104 | H | 1.00 | 0.007 | 1.00 | -1665268.00 |
| THR105 | H | 1.00 | 0.010 | 1.00 | -699960.00 |
| THR105 | HA | 0.79 | 0.013 | 1.00 | 0.19 |

3.104.8 Detailed Probabilities of VAL104HG11:

Overall probability: 0.814

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL104 | 0.74 | 1.00 |
| THR105 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| V104HA | 1.00 |
| V104HG12 | 1.00 |
| V104HG21 | 1.00 |
| V104H | 1.00 |
| V104HB | 1.00 |
| T105H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL104 | HA | 1.00 | 0.005 | 1.00 | 1.04 |
| VAL104 | HB | 1.00 | 0.012 | 1.00 | 3.14 |
| VAL104 | HG11 | 1.00 | 0.187 | 0.00 | 0.00 |
| VAL104 | HG21 | 1.00 | 0.033 | 0.70 | 0.00 |
| VAL104 | H | 1.00 | 0.028 | 1.00 | -1494884.00 |
| THR105 | H | 0.97 | 0.007 | 1.00 | -1485031.00 |
| THR105 | HA | 0.52 | 0.008 | 1.00 | 0.22 |

3.104.9 Detailed Probabilities of VAL104HG21:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL104 | 0.80 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| V104HA | 1.00 |
| V104HG11 | 1.00 |
| V104HG22 | 1.00 |
| V104H | 1.00 |
| V104HB | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL104 | HA | 1.00 | 0.029 | 1.00 | 1.04 |
| VAL104 | HB | 1.00 | 0.022 | 1.00 | 3.14 |
| VAL104 | HG11 | 1.00 | 0.153 | 0.00 | 0.00 |
| VAL104 | HG21 | 1.00 | 0.001 | 1.00 | 102.88 |
| VAL104 | H | 1.00 | 0.006 | 1.00 | -1494884.00 |

3.104.10 Detailed Probabilities of VAL104H:

Overall probability: 0.846

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| LEU103 | 1.00 | 1.00 |
| VAL104 | 0.60 | 1.00 |
| THR105 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| L103HA | 1.00 |
| L103H | 1.00 |
| L103HB3 | 1.00 |
| L103HG | 0.98 |
| L103HB2 | 1.00 |
| V104HA | 1.00 |
| V104HG11 | 1.00 |
| V104HG21 | 1.00 |
| V104HB | 1.00 |
| V104H | 1.00 |
| T105H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| LEU103 | HA | 1.00 | 0.007 | 1.00 | 0.66 |
| LEU103 | HB2 | 1.00 | 0.001 | 1.00 | 0.52 |
| LEU103 | HB3 | 1.00 | 0.002 | 1.00 | 0.47 |
| LEU103 | HG | 0.98 | 0.002 | 1.00 | 0.18 |
| LEU103 | H | 1.00 | 0.001 | 1.00 | -2261419.00 |
| LEU103 | HD11 | 0.55 | 0.017 | 1.00 | 0.14 |
| LEU103 | HD21 | 0.58 | 0.009 | 1.00 | 0.14 |
| VAL104 | HA | 1.00 | 0.062 | 0.00 | 0.00 |
| VAL104 | HB | 1.00 | 0.001 | 1.00 | 0.96 |
| VAL104 | HG11 | 1.00 | 0.281 | 0.00 | 0.00 |
| VAL104 | HG21 | 1.00 | 0.002 | 1.00 | 0.86 |
| VAL104 | H | 1.00 | 0.001 | 1.00 | -21124306.00 |
| THR105 | H | 1.00 | 0.006 | 1.00 | -307071.00 |

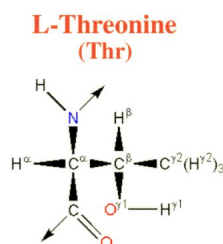
3.105 THR(105)

Figure 95: Image from the BMRB

Residue probability: 0.950

Residue probability confidence: 0.860

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 174.066 | 174.627 | 1.788 | 0.000 | 0.000 |
| CA 3.105.1 | 61.243 | 62.330 | 4.136 | 0.889 | 0.875 |
| CB 3.105.2 | 69.637 | 69.395 | 4.500 | 1.000 | 0.833 |
| CG2 3.105.3 | 21.734 | 21.588 | 1.595 | 1.000 | 0.833 |
| N 3.105.4 | 118.135 | 115.370 | 5.913 | 1.000 | 0.900 |
| HA 3.105.5 | 4.439 | 4.461 | 0.626 | 0.889 | 0.875 |
| HB 3.105.6 | 4.309 | 4.172 | 0.855 | 1.000 | 0.833 |
| HG2 3.105.7 | 1.201 | 1.134 | 0.349 | 1.000 | 0.833 |
| H 3.105.8 | 8.707 | 8.272 | 1.597 | 0.821 | 0.900 |
| HG1 | NA | – | – | 0.000 | 0.000 |

3.105.1 Detailed Probabilities of THR105CA:

Overall probability: 0.889

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL104 | 0.67 | 1.00 |
| THR105 | 1.00 | 0.80 |
| GLU106 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| V104HA | 1.00 |
| T105HB | 1.00 |
| T105HG21 | 1.00 |
| T105H | 1.00 |
| T105HG1 | 1.00 |
| T105HA | 1.00 |
| E106H | 1.00 |
| E106HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL104 | HA | 1.00 | 0.099 | 0.00 | 0.00 |
| VAL104 | HB | 0.79 | 0.013 | 1.00 | 0.19 |
| VAL104 | HG11 | 0.54 | 0.008 | 1.00 | 0.22 |
| THR105 | HA | 1.00 | 0.002 | 1.00 | 18.23 |
| THR105 | HB | 1.00 | 0.002 | 1.00 | 1.67 |
| THR105 | HG21 | 1.00 | 0.003 | 1.00 | 1.99 |
| THR105 | H | 1.00 | 0.000 | 1.00 | 0.77 |
| GLU106 | HA | 1.00 | 0.022 | 1.00 | 18.23 |
| GLU106 | H | 1.00 | 0.000 | 1.00 | 1.07 |

3.105.2 Detailed Probabilities of THR105CB:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR105 | 1.00 | 0.80 |
| GLU106 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| T105HA | 1.00 |
| T105HG21 | 1.00 |
| T105H | 1.00 |
| T105HG1 | 1.00 |
| T105HB | 1.00 |
| E106H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR105 | HA | 1.00 | 0.002 | 1.00 | 1.58 |
| THR105 | HB | 1.00 | 0.003 | 1.00 | 19.45 |
| THR105 | HG21 | 1.00 | 0.003 | 1.00 | 3.17 |
| THR105 | H | 1.00 | 0.000 | 1.00 | 0.59 |
| GLU106 | H | 1.00 | 0.005 | 1.00 | 0.41 |
| GLU106 | HA | 0.79 | 0.018 | 1.00 | 1.58 |

3.105.3 Detailed Probabilities of THR105CG2:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR105 | 1.00 | 0.80 |
| GLU106 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| T105HA | 1.00 |
| T105HB | 1.00 |
| T105HG22 | 1.00 |
| T105H | 1.00 |
| T105HG1 | 1.00 |
| E106H | 0.95 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR105 | HA | 1.00 | 0.024 | 1.00 | 2.96 |
| THR105 | HB | 1.00 | 0.002 | 1.00 | 2.98 |
| THR105 | HG21 | 1.00 | 0.001 | 1.00 | 231.85 |
| THR105 | H | 1.00 | 0.000 | 1.00 | 0.96 |
| GLU106 | H | 0.95 | 0.002 | 1.00 | 0.21 |

3.105.4 Detailed Probabilities of THR105N:

Overall probability: 1.000

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL104 | 1.00 | 1.00 |
| THR105 | 1.00 | 0.80 |
| GLU106 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| V104HA | 1.00 |
| V104H | 1.00 |
| V104HG11 | 0.97 |
| V104HB | 1.00 |
| T105HA | 1.00 |
| T105HB | 1.00 |
| T105HG21 | 1.00 |
| T105HG1 | 1.00 |
| T105H | 1.00 |
| E106H | 1.00 |

NOESY contacts detailed probability

3.105 THR(105)

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL104 | HA | 1.00 | 0.010 | 1.00 | -2603232.00 |
| VAL104 | HB | 1.00 | 0.010 | 1.00 | -699960.00 |
| VAL104 | HG11 | 0.97 | 0.007 | 1.00 | -1485031.00 |
| VAL104 | H | 1.00 | 0.006 | 1.00 | -307071.00 |
| VAL104 | HG21 | 0.94 | 0.027 | 1.00 | -1485031.00 |
| THR105 | HA | 1.00 | 0.004 | 1.00 | -972897.00 |
| THR105 | HB | 1.00 | 0.002 | 1.00 | -758658.00 |
| THR105 | HG21 | 1.00 | 0.004 | 1.00 | -1018454.00 |
| THR105 | H | 1.00 | 0.001 | 1.00 | -12094558.00 |
| GLU106 | H | 1.00 | 0.007 | 1.00 | -281604.00 |
| GLU106 | HA | 0.82 | 0.016 | 1.00 | -972897.00 |

3.105.5 Detailed Probabilities of THR105HA:

Overall probability: 0.889

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL104 | 0.50 | 1.00 |
| THR105 | 1.00 | 0.80 |
| GLU106 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| V104HA | 1.00 |
| T105HB | 1.00 |
| T105HG21 | 1.00 |
| T105H | 1.00 |
| T105HG1 | 1.00 |
| T105HA | 1.00 |
| E106H | 1.00 |
| E106HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL104 | HA | 1.00 | 0.069 | 0.00 | 0.00 |
| VAL104 | HB | 0.79 | 0.018 | 1.00 | 0.06 |
| THR105 | HA | 1.00 | 0.002 | 1.00 | 18.23 |
| THR105 | HB | 1.00 | 0.002 | 1.00 | 1.58 |
| THR105 | HG21 | 1.00 | 0.024 | 1.00 | 2.96 |
| THR105 | H | 1.00 | 0.004 | 1.00 | -972897.00 |
| GLU106 | HA | 1.00 | 0.022 | 1.00 | 55.95 |
| GLU106 | H | 1.00 | 0.010 | 1.00 | -3430141.00 |
| GLU106 | HB2 | 0.56 | 0.020 | 1.00 | 1.00 |

3.105.6 Detailed Probabilities of THR105HB:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR105 | 1.00 | 0.80 |
| GLU106 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| T105HA | 1.00 |
| T105HG21 | 1.00 |
| T105H | 1.00 |
| T105HG1 | 1.00 |
| T105HB | 1.00 |
| E106H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR105 | HA | 1.00 | 0.002 | 1.00 | 1.67 |
| THR105 | HB | 1.00 | 0.003 | 1.00 | 19.45 |
| THR105 | HG21 | 1.00 | 0.002 | 1.00 | 2.98 |
| THR105 | H | 1.00 | 0.002 | 1.00 | -758658.00 |
| GLU106 | H | 1.00 | 0.000 | 1.00 | -987712.00 |

3.105.7 Detailed Probabilities of THR105HG21:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR105 | 1.00 | 0.80 |
| GLU106 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| T105HA | 1.00 |
| T105HB | 1.00 |
| T105HG22 | 1.00 |
| T105H | 1.00 |
| T105HG1 | 1.00 |
| E106H | 0.95 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR105 | HA | 1.00 | 0.003 | 1.00 | 1.99 |
| THR105 | HB | 1.00 | 0.003 | 1.00 | 3.17 |
| THR105 | HG21 | 1.00 | 0.001 | 1.00 | 231.85 |
| THR105 | H | 1.00 | 0.004 | 1.00 | -1018454.00 |
| GLU106 | H | 0.95 | 0.004 | 1.00 | -611818.00 |

3.105.8 Detailed Probabilities of THR105H:

Overall probability: 0.821

Overall confidence: 0.900

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| VAL104 | 0.61 | 1.00 |
| THR105 | 1.00 | 0.80 |
| GLU106 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| V104HA | 1.00 |
| V104H | 1.00 |
| V104HG11 | 0.97 |
| V104HB | 1.00 |
| T105HA | 1.00 |
| T105HB | 1.00 |
| T105HG21 | 1.00 |
| T105HG1 | 1.00 |
| T105H | 1.00 |
| E106H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| VAL104 | HA | 1.00 | 0.094 | 0.00 | 0.00 |
| VAL104 | HB | 1.00 | 0.001 | 1.00 | 0.34 |
| VAL104 | HG11 | 0.97 | 0.110 | 0.03 | 0.00 |
| VAL104 | H | 1.00 | 0.003 | 1.00 | -208312.00 |
| VAL104 | HG21 | 0.94 | 0.000 | 1.00 | 0.37 |
| THR105 | HA | 1.00 | 0.000 | 1.00 | 0.77 |
| THR105 | HB | 1.00 | 0.000 | 1.00 | 0.59 |
| THR105 | HG21 | 1.00 | 0.000 | 1.00 | 0.96 |
| THR105 | H | 1.00 | 0.001 | 1.00 | -12094558.00 |
| GLU106 | H | 1.00 | 0.001 | 1.00 | -617193.00 |
| GLU106 | HA | 0.82 | 0.022 | 1.00 | 0.09 |

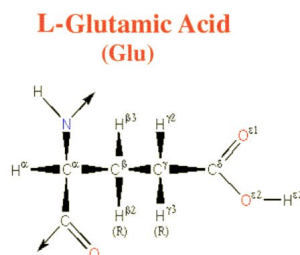
3.106 GLU(106)

Figure 96: Image from the BMRB

Residue probability: 0.905

Residue probability confidence: 0.908

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | 175.028 | 176.942 | 2.547 | 0.000 | 0.000 |
| CA 3.106.1 | 56.232 | 57.442 | 3.837 | 1.000 | 1.000 |
| CB 3.106.2 | 30.613 | 30.185 | 4.018 | 0.857 | 0.875 |
| CG 3.106.3 | 36.010 | 36.085 | 1.533 | 0.857 | 0.875 |
| N 3.106.4 | 122.946 | 120.574 | 4.837 | 1.000 | 0.917 |
| HA 3.106.5 | 4.419 | 4.245 | 0.429 | 1.000 | 1.000 |
| HB2 3.106.6 | 2.154 | 2.021 | 0.233 | 0.714 | 0.875 |
| HB3 3.106.7 | 1.949 | 1.994 | 0.244 | 0.857 | 0.875 |
| HG2 3.106.8 | 2.281 | 2.258 | 0.226 | 1.000 | 0.875 |
| HG3 3.106.9 | 2.310 | 2.233 | 0.232 | 1.000 | 0.875 |
| H 3.106.10 | 8.438 | 8.332 | 0.601 | 0.769 | 0.917 |
| HE2 | NA | - | - | 0.000 | 0.000 |

3.106.1 Detailed Probabilities of GLU106CA:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR105 | 1.00 | 1.00 |
| GLU106 | 1.00 | 1.00 |
| GLU107 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T105HA | 1.00 |
| E106HB2 | 1.00 |
| E106HB3 | 1.00 |
| E106HG2 | 1.00 |
| E106HG3 | 1.00 |
| E106H | 1.00 |
| E106HA | 1.00 |
| E107H | 1.00 |
| E107HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR105 | HA | 1.00 | 0.022 | 1.00 | 55.95 |
| THR105 | H | 0.82 | 0.022 | 1.00 | 0.09 |
| GLU106 | HA | 1.00 | 0.002 | 1.00 | 55.95 |
| GLU106 | HB2 | 1.00 | 0.001 | 1.00 | 1.95 |
| GLU106 | HB3 | 1.00 | 0.006 | 1.00 | 1.99 |
| GLU106 | HG2 | 1.00 | 0.000 | 1.00 | 0.91 |
| GLU106 | HG3 | 1.00 | 0.029 | 1.00 | 0.91 |
| GLU106 | H | 1.00 | 0.003 | 1.00 | 0.48 |
| GLU107 | HA | 1.00 | 0.002 | 1.00 | 0.19 |
| GLU107 | H | 1.00 | 0.001 | 1.00 | 3.52 |

3.106.2 Detailed Probabilities of GLU106CB:

Overall probability: 0.857

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU106 | 1.00 | 0.86 |
| GLU107 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E106HA | 1.00 |
| E106HB2 | 1.00 |
| E106HG2 | 1.00 |
| E106HG3 | 1.00 |
| E106H | 1.00 |
| E106HE2 | 1.00 |
| E106HB3 | 1.00 |
| E107H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU106 | HA | 1.00 | 0.000 | 1.00 | 0.87 |
| GLU106 | HB2 | 1.00 | 0.004 | 1.00 | 9.75 |
| GLU106 | HB3 | 1.00 | 0.001 | 1.00 | 29.96 |
| GLU106 | HG2 | 1.00 | 0.022 | 1.00 | 1.72 |
| GLU106 | HG3 | 1.00 | 0.007 | 1.00 | 1.72 |
| GLU106 | H | 1.00 | 0.007 | 1.00 | 0.37 |
| GLU107 | H | 1.00 | 0.315 | 0.00 | 0.00 |

3.106.3 Detailed Probabilities of GLU106CG:

Overall probability: 0.857

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU106 | 0.83 | 0.86 |
| GLU107 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E106HA | 1.00 |
| E106HB2 | 1.00 |
| E106HB3 | 1.00 |
| E106HG3 | 1.00 |
| E106H | 1.00 |
| E106HE2 | 1.00 |
| E106HG2 | 1.00 |
| E107H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU106 | HA | 1.00 | 0.001 | 1.00 | 0.61 |
| GLU106 | HB2 | 1.00 | 0.002 | 1.00 | 2.80 |
| GLU106 | HB3 | 1.00 | 0.010 | 1.00 | 3.06 |
| GLU106 | HG2 | 1.00 | 0.008 | 1.00 | 51.74 |
| GLU106 | HG3 | 1.00 | 0.021 | 1.00 | 51.53 |
| GLU106 | H | 1.00 | 0.043 | 0.00 | 0.00 |
| GLU107 | H | 0.98 | 0.001 | 1.00 | 0.13 |

3.106.4 Detailed Probabilities of GLU106N:

Overall probability: 1.000

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR105 | 1.00 | 0.80 |
| GLU106 | 1.00 | 1.00 |
| GLU107 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| T105HA | 1.00 |
| T105HG23 | 0.95 |
| T105H | 1.00 |
| T105HB | 1.00 |
| T105HG1 | 0.98 |
| E106HA | 1.00 |
| E106HB2 | 1.00 |
| E106HB3 | 1.00 |
| E106HG2 | 1.00 |
| E106HG3 | 1.00 |
| E106H | 1.00 |
| E107H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR105 | HA | 1.00 | 0.010 | 1.00 | -3430141.00 |
| THR105 | HB | 1.00 | 0.000 | 1.00 | -987712.00 |
| THR105 | HG21 | 0.95 | 0.004 | 1.00 | -611818.00 |
| THR105 | H | 1.00 | 0.001 | 1.00 | -617193.00 |
| GLU106 | HA | 1.00 | 0.010 | 1.00 | -3430141.00 |
| GLU106 | HB2 | 1.00 | 0.006 | 1.00 | -666392.00 |
| GLU106 | HB3 | 1.00 | 0.001 | 1.00 | -1441601.00 |
| GLU106 | HG2 | 1.00 | 0.006 | 1.00 | -552641.00 |
| GLU106 | HG3 | 1.00 | 0.023 | 1.00 | -552641.00 |
| GLU106 | H | 1.00 | 0.000 | 1.00 | -8502220.00 |
| GLU107 | H | 1.00 | 0.004 | 1.00 | -435281.00 |

3.106.5 Detailed Probabilities of GLU106HA:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR105 | 1.00 | 1.00 |
| GLU106 | 1.00 | 1.00 |
| GLU107 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| T105HA | 1.00 |
| E106HB2 | 1.00 |
| E106HB3 | 1.00 |
| E106HG2 | 1.00 |
| E106HG3 | 1.00 |
| E106H | 1.00 |
| E106HA | 1.00 |
| E107H | 1.00 |
| E107HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR105 | HA | 1.00 | 0.022 | 1.00 | 18.23 |
| THR105 | HB | 0.79 | 0.018 | 1.00 | 1.58 |
| THR105 | H | 0.82 | 0.016 | 1.00 | -972897.00 |
| GLU106 | HA | 1.00 | 0.002 | 1.00 | 55.95 |
| GLU106 | HB2 | 1.00 | 0.000 | 1.00 | 1.00 |
| GLU106 | HB3 | 1.00 | 0.000 | 1.00 | 0.87 |
| GLU106 | HG2 | 1.00 | 0.001 | 1.00 | 0.61 |
| GLU106 | HG3 | 1.00 | 0.001 | 1.00 | 0.61 |
| GLU106 | H | 1.00 | 0.010 | 1.00 | -3430141.00 |
| GLU107 | HA | 1.00 | 0.006 | 1.00 | 0.11 |
| GLU107 | H | 1.00 | 0.002 | 1.00 | -7678076.00 |

3.106.6 Detailed Probabilities of GLU106HB2:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU106 | 0.83 | 0.86 |
| GLU107 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E106HA | 1.00 |
| E106HB3 | 1.00 |
| E106HG2 | 1.00 |
| E106HG3 | 1.00 |
| E106H | 1.00 |
| E106HE2 | 1.00 |
| E106HB2 | 1.00 |
| E107H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU106 | HA | 1.00 | 0.001 | 1.00 | 1.95 |
| GLU106 | HB2 | 1.00 | 0.139 | 0.00 | 0.00 |
| GLU106 | HB3 | 1.00 | 0.004 | 1.00 | 9.75 |
| GLU106 | HG2 | 1.00 | 0.002 | 1.00 | 2.80 |
| GLU106 | HG3 | 1.00 | 0.002 | 1.00 | 2.80 |
| GLU106 | H | 1.00 | 0.006 | 1.00 | -666392.00 |
| GLU107 | H | 1.00 | 0.046 | 0.00 | 0.00 |

3.106.7 Detailed Probabilities of GLU106HB3:

Overall probability: 0.857

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU106 | 1.00 | 0.86 |
| GLU107 | 0.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E106HA | 1.00 |
| E106HB2 | 1.00 |
| E106HG2 | 1.00 |
| E106HG3 | 1.00 |
| E106H | 1.00 |
| E106HE2 | 1.00 |
| E106HB3 | 1.00 |
| E107H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU106 | HA | 1.00 | 0.006 | 1.00 | 1.99 |
| GLU106 | HB2 | 1.00 | 0.001 | 1.00 | 9.15 |
| GLU106 | HB3 | 1.00 | 0.001 | 1.00 | 29.96 |
| GLU106 | HG2 | 1.00 | 0.010 | 1.00 | 3.06 |
| GLU106 | HG3 | 1.00 | 0.010 | 1.00 | 3.06 |
| GLU106 | H | 1.00 | 0.001 | 1.00 | -1441601.00 |
| GLU107 | H | 1.00 | 0.041 | 0.00 | 0.00 |

3.106.8 Detailed Probabilities of GLU106HG2:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU106 | 1.00 | 0.86 |
| GLU107 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E106HA | 1.00 |
| E106HB2 | 1.00 |
| E106HB3 | 1.00 |
| E106HG3 | 1.00 |
| E106H | 1.00 |
| E106HE2 | 1.00 |
| E106HG2 | 1.00 |
| E107H | 0.98 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU106 | HA | 1.00 | 0.000 | 1.00 | 0.91 |
| GLU106 | HB2 | 1.00 | 0.012 | 1.00 | 3.78 |
| GLU106 | HB3 | 1.00 | 0.022 | 1.00 | 1.72 |
| GLU106 | HG2 | 1.00 | 0.008 | 1.00 | 51.74 |
| GLU106 | HG3 | 1.00 | 0.008 | 1.00 | 51.74 |
| GLU106 | H | 1.00 | 0.006 | 1.00 | -552641.00 |
| GLU107 | H | 0.98 | 0.025 | 1.00 | -429440.00 |

3.106.9 Detailed Probabilities of GLU106HG3:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU106 | 1.00 | 0.86 |
| GLU107 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E106HA | 1.00 |
| E106HB2 | 1.00 |
| E106HB3 | 1.00 |
| E106HG2 | 1.00 |
| E106H | 1.00 |
| E106HE2 | 1.00 |
| E106HG3 | 1.00 |
| E107H | 0.97 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU106 | HA | 1.00 | 0.029 | 1.00 | 0.91 |
| GLU106 | HB2 | 1.00 | 0.017 | 1.00 | 3.78 |
| GLU106 | HB3 | 1.00 | 0.007 | 1.00 | 1.72 |
| GLU106 | HG2 | 1.00 | 0.021 | 1.00 | 51.53 |
| GLU106 | HG3 | 1.00 | 0.021 | 1.00 | 51.53 |
| GLU106 | H | 1.00 | 0.023 | 1.00 | -552641.00 |
| GLU107 | H | 0.97 | 0.004 | 1.00 | -429440.00 |

3.106.10 Detailed Probabilities of GLU106H:

Overall probability: 0.769

Overall confidence: 0.917

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| THR105 | 1.00 | 0.80 |
| GLU106 | 0.50 | 1.00 |
| GLU107 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|----------|----------------------|
| T105HA | 1.00 |
| T105HG23 | 0.95 |
| T105H | 1.00 |
| T105HB | 1.00 |
| T105HG1 | 0.98 |
| E106HA | 1.00 |
| E106HB2 | 1.00 |
| E106HB3 | 1.00 |
| E106HG2 | 1.00 |
| E106HG3 | 1.00 |
| E106H | 1.00 |
| E107H | 1.00 |

NOESY contacts detailed probability

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| THR105 | HA | 1.00 | 0.000 | 1.00 | 1.07 |
| THR105 | HB | 1.00 | 0.005 | 1.00 | 0.41 |
| THR105 | HG21 | 0.95 | 0.002 | 1.00 | 0.21 |
| THR105 | H | 1.00 | 0.007 | 1.00 | -281604.00 |
| GLU106 | HA | 1.00 | 0.003 | 1.00 | 0.48 |
| GLU106 | HB2 | 1.00 | 0.311 | 0.00 | 0.00 |
| GLU106 | HB3 | 1.00 | 0.007 | 1.00 | 0.37 |
| GLU106 | HG2 | 1.00 | 0.043 | 0.00 | 0.00 |
| GLU106 | HG3 | 1.00 | 0.043 | 0.00 | 0.00 |
| GLU106 | H | 1.00 | 0.000 | 1.00 | -8502220.00 |
| GLU107 | H | 1.00 | 0.004 | 1.00 | -468969.00 |
| GLU107 | HA | 0.88 | 0.005 | 1.00 | 0.06 |
| GLU107 | HB2 | 0.67 | 0.007 | 1.00 | 0.37 |

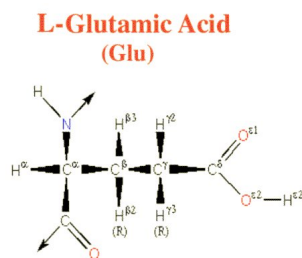


Figure 97: Image from the BMRB

Residue probability: 0.833
Residue probability confidence: 0.914

Chemical Shift Distributions and Assignment Probabilities

| Atom | Assigned CS | DB avg. | DB std | Overall probability | Overall confidence |
|-------------|-------------|---------|--------|---------------------|--------------------|
| C | NA | – | – | 0.000 | 0.000 |
| CA 3.107.1 | 58.046 | 57.442 | 3.837 | 1.000 | 1.000 |
| CB 3.107.2 | 31.124 | 30.185 | 4.018 | 0.667 | 0.857 |
| CG 3.107.3 | 36.717 | 36.085 | 1.533 | 0.833 | 0.857 |
| N 3.107.4 | 126.458 | 120.574 | 4.837 | 0.833 | 1.000 |
| HA 3.107.5 | 4.115 | 4.245 | 0.429 | 1.000 | 1.000 |
| HB2 3.107.6 | 1.903 | 2.021 | 0.233 | 0.667 | 0.857 |
| HB3 3.107.7 | 2.067 | 1.994 | 0.244 | 0.833 | 0.857 |
| HG2 3.107.8 | 2.220 | 2.258 | 0.226 | 0.833 | 0.857 |
| HG3 3.107.9 | 2.218 | 2.233 | 0.232 | 0.833 | 0.857 |
| H 3.107.10 | 8.130 | 8.332 | 0.601 | 0.833 | 1.000 |
| HE2 | NA | – | – | 0.000 | 0.000 |

3.107.1 Detailed Probabilities of GLU107CA:

Overall probability: 1.000
Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU106 | 1.00 | 1.00 |
| GLU107 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E106HA | 1.00 |
| E107HB2 | 1.00 |
| E107HB3 | 1.00 |
| E107HG2 | 1.00 |
| E107HG3 | 1.00 |
| E107H | 1.00 |
| E107HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU106 | HA | 1.00 | 0.006 | 1.00 | 0.11 |
| GLU106 | H | 0.88 | 0.005 | 1.00 | 0.06 |
| GLU107 | HA | 1.00 | 0.002 | 1.00 | 76.91 |
| GLU107 | HB2 | 1.00 | 0.004 | 1.00 | 0.82 |
| GLU107 | HB3 | 1.00 | 0.003 | 1.00 | 1.14 |
| GLU107 | HG2 | 1.00 | 0.008 | 1.00 | 0.76 |
| GLU107 | HG3 | 1.00 | 0.006 | 1.00 | 0.76 |
| GLU107 | H | 1.00 | 0.001 | 1.00 | 1.06 |

3.107.2 Detailed Probabilities of GLU107CB:

Overall probability: 0.667

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU107 | 0.67 | 0.86 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E107HA | 1.00 |
| E107HB3 | 1.00 |
| E107HG2 | 1.00 |
| E107HG3 | 1.00 |
| E107H | 1.00 |
| E107HE2 | 1.00 |
| E107HB2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU107 | HA | 1.00 | 0.005 | 1.00 | 0.65 |
| GLU107 | HB2 | 1.00 | 0.002 | 1.00 | 92.80 |
| GLU107 | HB3 | 1.00 | 0.003 | 1.00 | 11.32 |
| GLU107 | HG2 | 1.00 | 0.070 | 0.00 | 0.00 |
| GLU107 | HG3 | 1.00 | 0.068 | 0.00 | 0.00 |
| GLU107 | H | 1.00 | 0.000 | 1.00 | 0.98 |

3.107.3 Detailed Probabilities of GLU107CG:

Overall probability: 0.833

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU107 | 0.83 | 0.86 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E107HA | 1.00 |
| E107HB2 | 1.00 |
| E107HB3 | 1.00 |
| E107HG2 | 1.00 |
| E107H | 1.00 |
| E107HE2 | 1.00 |
| E107HG3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU107 | HA | 1.00 | 0.008 | 1.00 | 0.67 |
| GLU107 | HB2 | 1.00 | 0.044 | 0.00 | 0.00 |
| GLU107 | HB3 | 1.00 | 0.004 | 1.00 | 8.98 |
| GLU107 | HG2 | 1.00 | 0.000 | 1.00 | 180.23 |
| GLU107 | HG3 | 1.00 | 0.002 | 1.00 | 180.23 |
| GLU107 | H | 1.00 | 0.001 | 1.00 | 0.63 |

3.107.4 Detailed Probabilities of GLU107N:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU106 | 0.67 | 1.00 |
| GLU107 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E106HG2 | 0.98 |
| E106HA | 1.00 |
| E106H | 1.00 |
| E106HB3 | 1.00 |
| E106HG3 | 0.97 |
| E106HB2 | 1.00 |
| E107HA | 1.00 |
| E107HB2 | 1.00 |
| E107HB3 | 1.00 |
| E107HG2 | 1.00 |
| E107HG3 | 1.00 |
| E107H | 1.00 |

NOESY contacts detailed probability

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| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU106 | HA | 1.00 | 0.002 | 1.00 | -7678076.00 |
| GLU106 | HB2 | 1.00 | 0.046 | 0.00 | 0.00 |
| GLU106 | HB3 | 1.00 | 0.041 | 0.00 | 0.00 |
| GLU106 | HG2 | 0.98 | 0.025 | 1.00 | -429440.00 |
| GLU106 | HG3 | 0.97 | 0.004 | 1.00 | -429440.00 |
| GLU106 | H | 1.00 | 0.004 | 1.00 | -468969.00 |
| GLU107 | HA | 1.00 | 0.002 | 1.00 | -2236162.00 |
| GLU107 | HB2 | 1.00 | 0.005 | 1.00 | -2772170.00 |
| GLU107 | HB3 | 1.00 | 0.004 | 1.00 | -1027469.00 |
| GLU107 | HG2 | 1.00 | 0.020 | 1.00 | -1596018.00 |
| GLU107 | HG3 | 1.00 | 0.018 | 1.00 | -1596018.00 |
| GLU107 | H | 1.00 | 0.003 | 1.00 | -91282752.00 |

3.107.5 Detailed Probabilities of GLU107HA:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU106 | 1.00 | 1.00 |
| GLU107 | 1.00 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E106HA | 1.00 |
| E107HB2 | 1.00 |
| E107HB3 | 1.00 |
| E107HG2 | 1.00 |
| E107HG3 | 1.00 |
| E107H | 1.00 |
| E107HA | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU106 | HA | 1.00 | 0.002 | 1.00 | 0.19 |
| GLU107 | HA | 1.00 | 0.002 | 1.00 | 76.91 |
| GLU107 | HB2 | 1.00 | 0.005 | 1.00 | 0.65 |
| GLU107 | HB3 | 1.00 | 0.003 | 1.00 | 0.88 |
| GLU107 | HG2 | 1.00 | 0.008 | 1.00 | 0.67 |
| GLU107 | HG3 | 1.00 | 0.008 | 1.00 | 0.67 |
| GLU107 | H | 1.00 | 0.002 | 1.00 | -2236162.00 |

3.107.6 Detailed Probabilities of GLU107HB2:

Overall probability: 0.667

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU107 | 0.67 | 0.86 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E107HA | 1.00 |
| E107HB3 | 1.00 |
| E107HG2 | 1.00 |
| E107HG3 | 1.00 |
| E107H | 1.00 |
| E107HE2 | 1.00 |
| E107HB2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU107 | HA | 1.00 | 0.004 | 1.00 | 0.82 |
| GLU107 | HB2 | 1.00 | 0.002 | 1.00 | 92.80 |
| GLU107 | HB3 | 1.00 | 0.000 | 1.00 | 12.83 |
| GLU107 | HG2 | 1.00 | 0.044 | 0.00 | 0.00 |
| GLU107 | HG3 | 1.00 | 0.044 | 0.00 | 0.00 |
| GLU107 | H | 1.00 | 0.005 | 1.00 | -2772170.00 |

3.107.7 Detailed Probabilities of GLU107HB3:

Overall probability: 0.833

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU107 | 0.83 | 0.86 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E107HA | 1.00 |
| E107HB2 | 1.00 |
| E107HG2 | 1.00 |
| E107HG3 | 1.00 |
| E107H | 1.00 |
| E107HE2 | 1.00 |
| E107HB3 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU107 | HA | 1.00 | 0.003 | 1.00 | 1.14 |
| GLU107 | HB2 | 1.00 | 0.003 | 1.00 | 11.32 |
| GLU107 | HB3 | 1.00 | 0.138 | 0.00 | 0.00 |
| GLU107 | HG2 | 1.00 | 0.004 | 1.00 | 8.98 |
| GLU107 | HG3 | 1.00 | 0.004 | 1.00 | 8.98 |
| GLU107 | H | 1.00 | 0.004 | 1.00 | -1027469.00 |

3.107.8 Detailed Probabilities of GLU107HG2:

Overall probability: 0.833

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU107 | 0.83 | 0.86 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E107HA | 1.00 |
| E107HB2 | 1.00 |
| E107HB3 | 1.00 |
| E107HG3 | 1.00 |
| E107H | 1.00 |
| E107HE2 | 1.00 |
| E107HG2 | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU107 | HA | 1.00 | 0.008 | 1.00 | 0.76 |
| GLU107 | HB2 | 1.00 | 0.070 | 0.00 | 0.00 |
| GLU107 | HB3 | 1.00 | 0.015 | 1.00 | 5.49 |
| GLU107 | HG2 | 1.00 | 0.000 | 1.00 | 180.23 |
| GLU107 | HG3 | 1.00 | 0.000 | 1.00 | 180.23 |
| GLU107 | H | 1.00 | 0.020 | 1.00 | -1596018.00 |

3.107.9 Detailed Probabilities of GLU107HG3:

Overall probability: 0.833

Overall confidence: 0.857

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU107 | 0.83 | 0.86 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E107HA | 1.00 |
| E107HB2 | 1.00 |
| E107HB3 | 1.00 |
| E107HG2 | 1.00 |
| E107H | 1.00 |
| E107HE2 | 1.00 |
| E107HG3 | 1.00 |

NOESY contacts detailed probability

3.107 *GLU(107)*

Areca @ NMRFAM

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU107 | HA | 1.00 | 0.006 | 1.00 | 0.76 |
| GLU107 | HB2 | 1.00 | 0.068 | 0.00 | 0.00 |
| GLU107 | HB3 | 1.00 | 0.013 | 1.00 | 5.49 |
| GLU107 | HG2 | 1.00 | 0.002 | 1.00 | 180.23 |
| GLU107 | HG3 | 1.00 | 0.002 | 1.00 | 180.23 |
| GLU107 | H | 1.00 | 0.018 | 1.00 | -1596018.00 |

3.107.10 Detailed Probabilities of GLU107H:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

| Residue | Probability | Confidence |
|---------|-------------|------------|
| GLU106 | 0.83 | 1.00 |
| GLU107 | 0.83 | 1.00 |

Expected NOESY Contacts

| Proton | Expected probability |
|---------|----------------------|
| E106HG2 | 0.98 |
| E106HA | 1.00 |
| E106H | 1.00 |
| E106HB3 | 1.00 |
| E106HG3 | 0.97 |
| E106HB2 | 1.00 |
| E107HA | 1.00 |
| E107HB2 | 1.00 |
| E107HB3 | 1.00 |
| E107HG2 | 1.00 |
| E107HG3 | 1.00 |
| E107H | 1.00 |

NOESY contacts detailed probability

| Residue | Proton | Expected probability | Min PPM differences | Probability | Peak intensity ratio |
|---------|--------|----------------------|---------------------|-------------|----------------------|
| GLU106 | HA | 1.00 | 0.001 | 1.00 | 3.52 |
| GLU106 | HB2 | 1.00 | 0.003 | 1.00 | 0.27 |
| GLU106 | HB3 | 1.00 | 0.315 | 0.00 | 0.00 |
| GLU106 | HG2 | 0.98 | 0.001 | 1.00 | 0.13 |
| GLU106 | HG3 | 0.97 | 0.001 | 1.00 | 0.13 |
| GLU106 | H | 1.00 | 0.004 | 1.00 | -435281.00 |
| GLU107 | HA | 1.00 | 0.001 | 1.00 | 1.06 |
| GLU107 | HB2 | 1.00 | 0.000 | 1.00 | 0.98 |
| GLU107 | HB3 | 1.00 | 2.457 | 0.00 | 0.00 |
| GLU107 | HG2 | 1.00 | 0.001 | 1.00 | 0.63 |
| GLU107 | HG3 | 1.00 | 0.001 | 1.00 | 0.63 |
| GLU107 | H | 1.00 | 0.003 | 1.00 | -91282752.00 |