

# 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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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](mailto:ARECA.nmrfam@gmail.com).

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## 2 Overall Reports

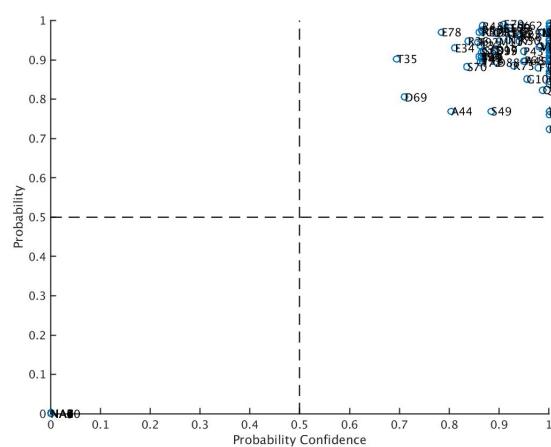
Figure: Overall 2D probabilities v.s. confidences2.1

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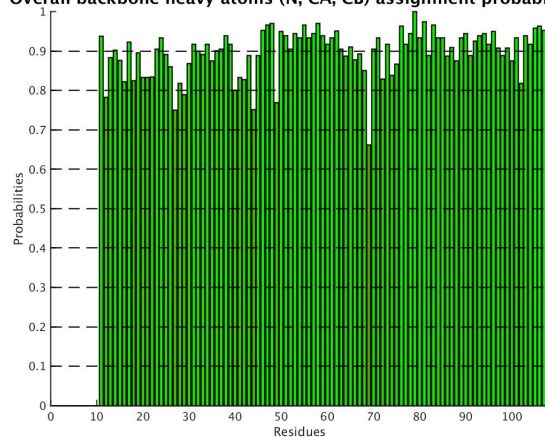
## 2.1 Overall 2D probabilities v.s. confidences

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

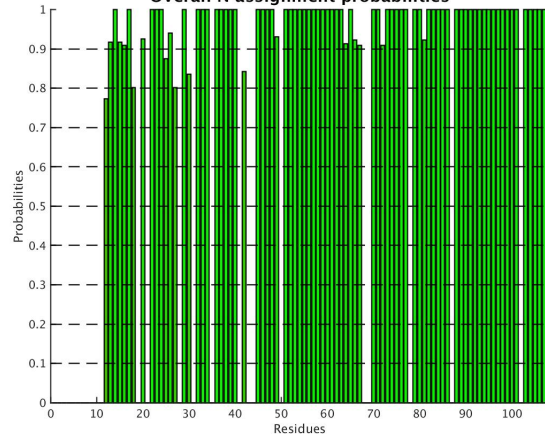


## 2.2 Figures: Overall Probabilities

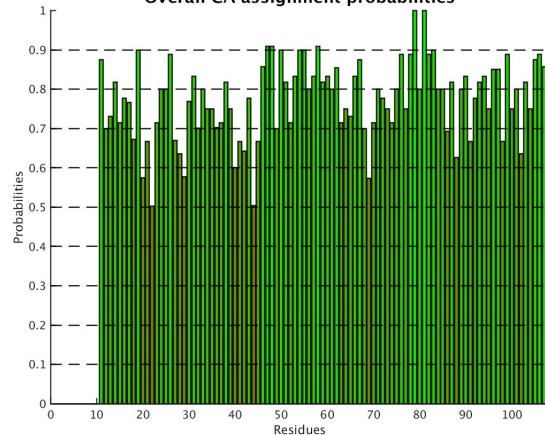
Overall backbone heavy atoms (N, CA, CB) assignment probabilities

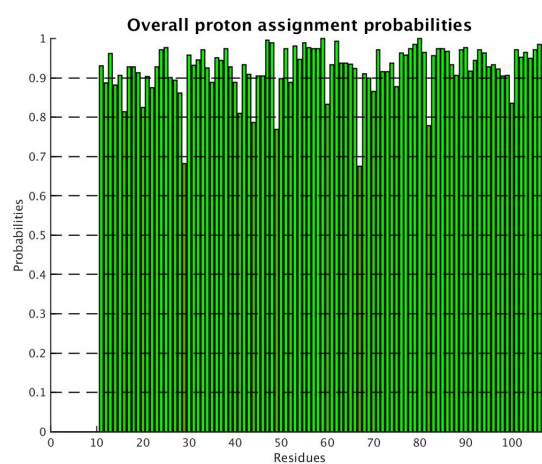
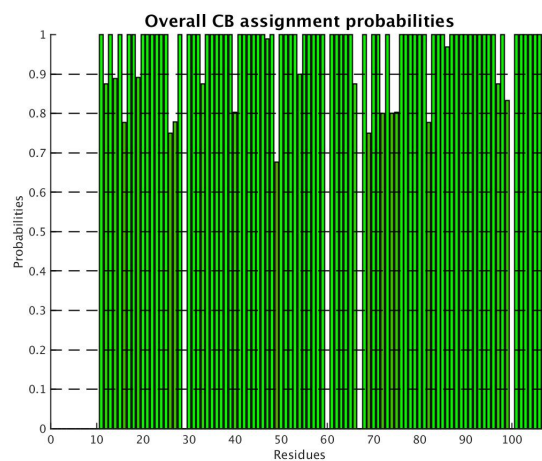


Overall N assignment probabilities

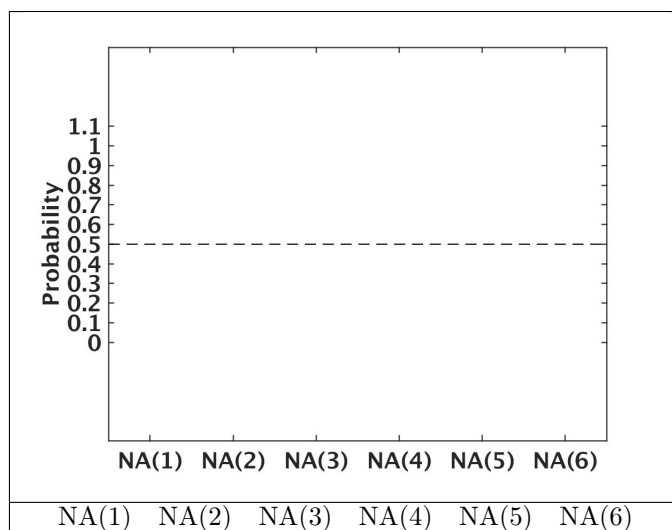


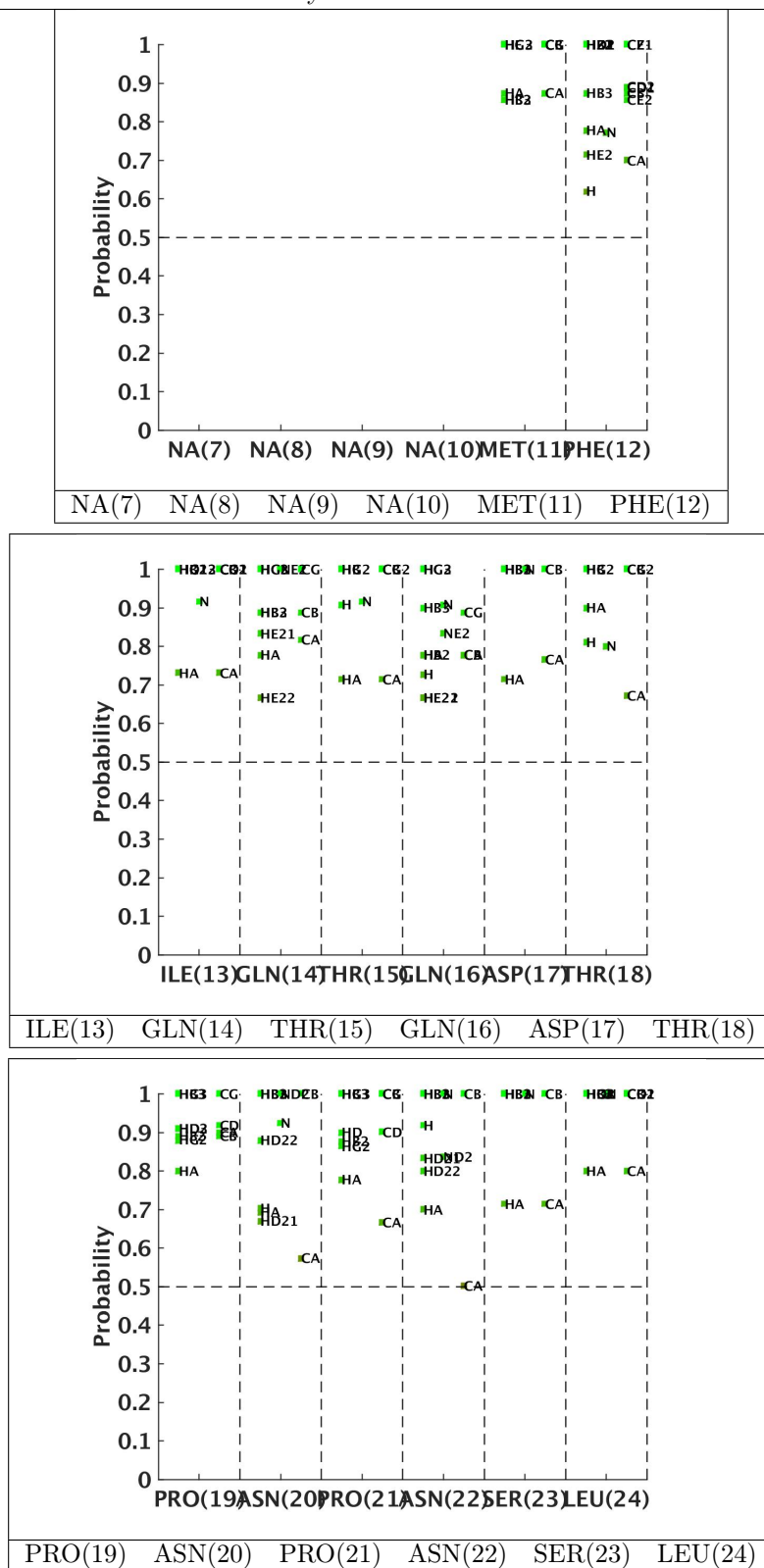
Overall CA assignment probabilities

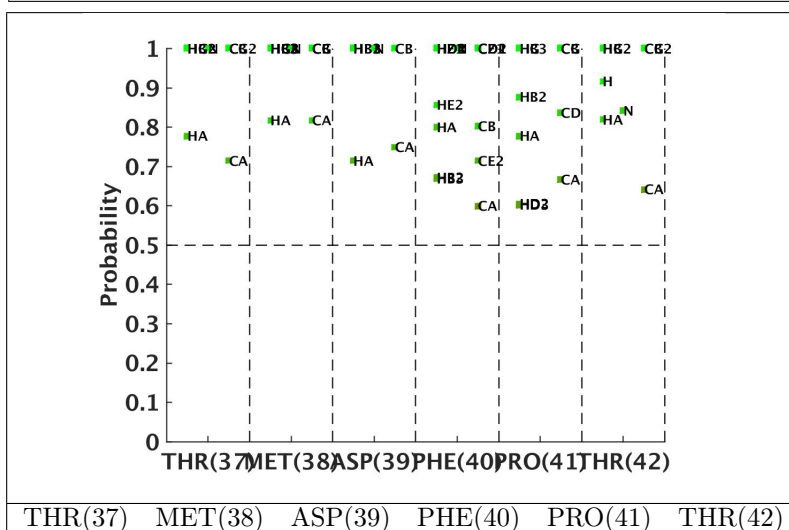
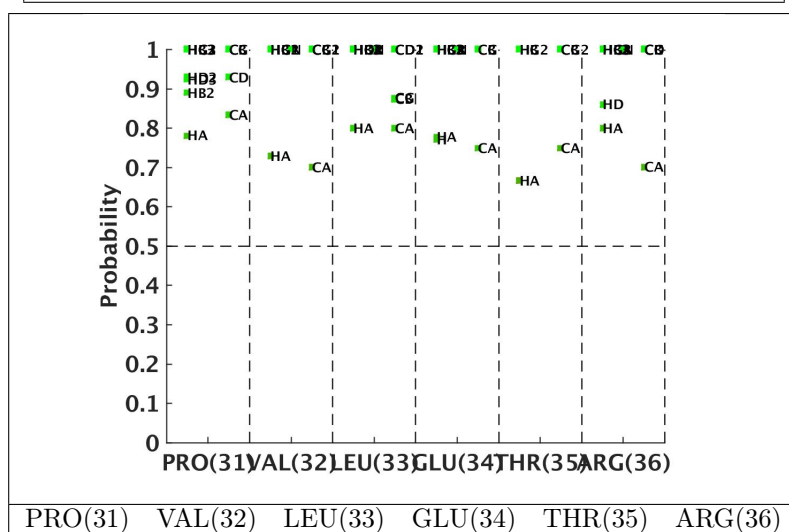
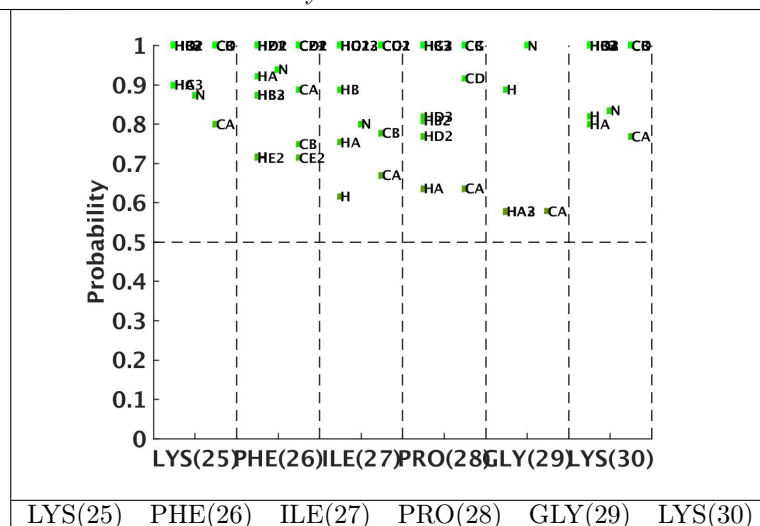


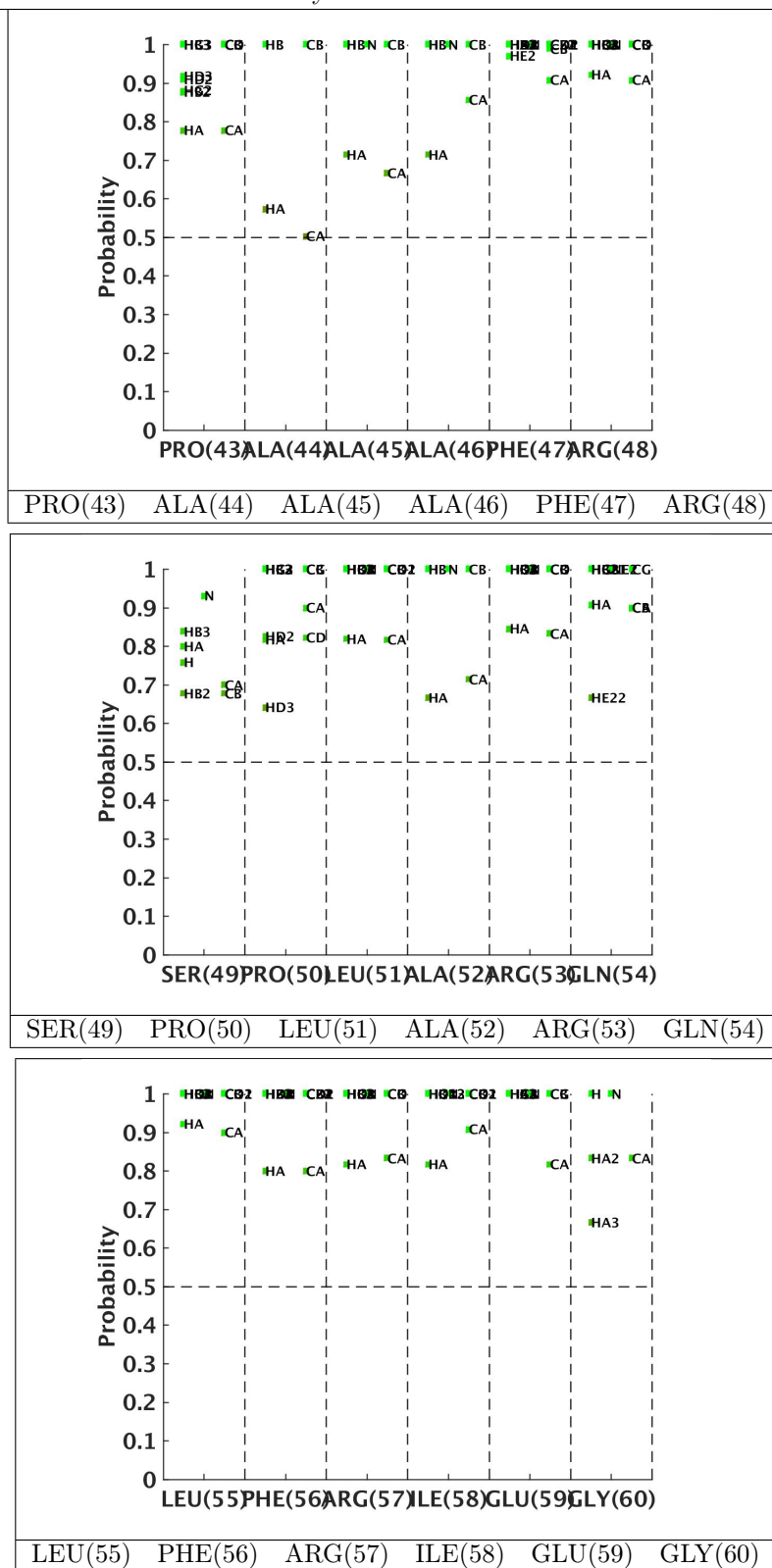


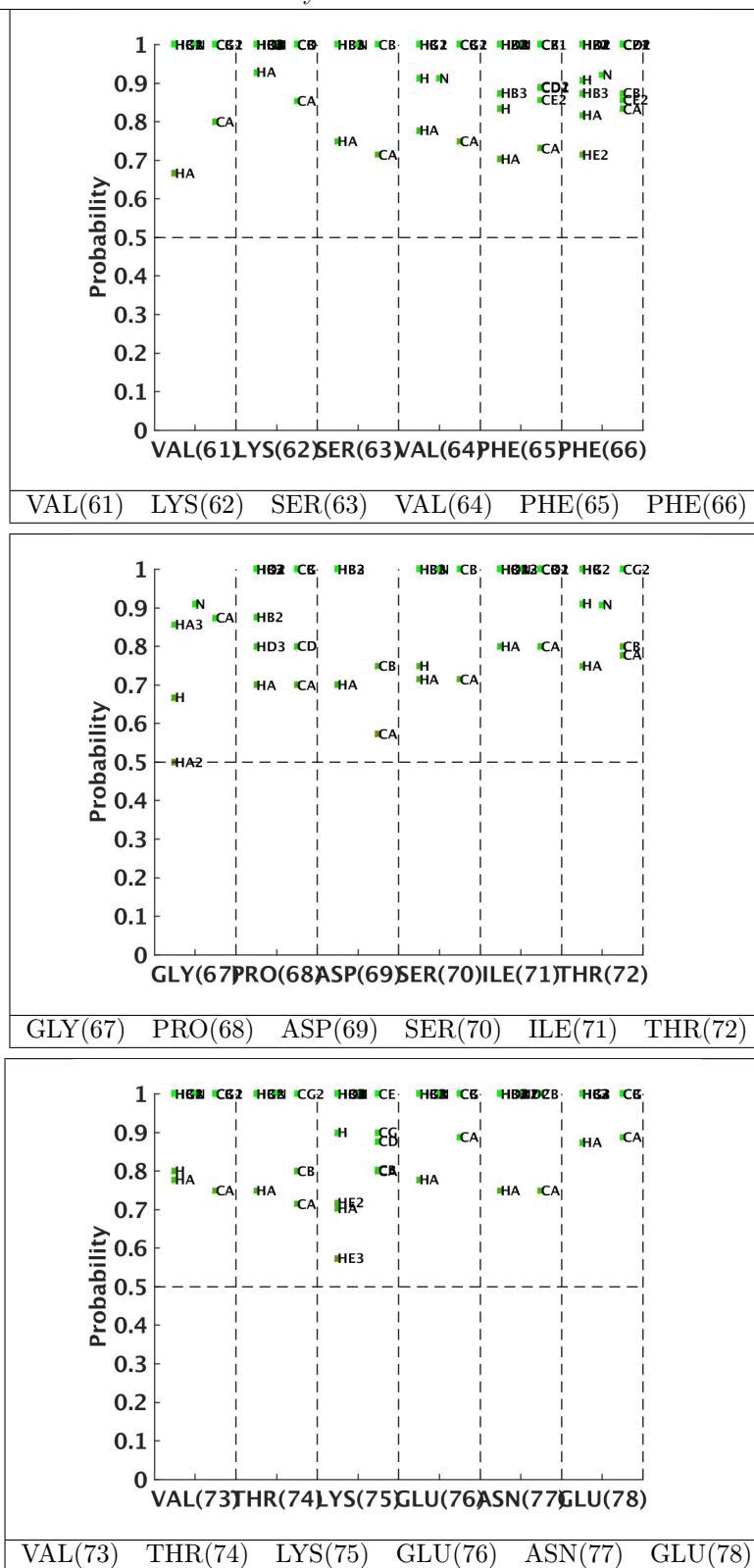
## 2.3 Figures: Probabilities of atoms for every residue

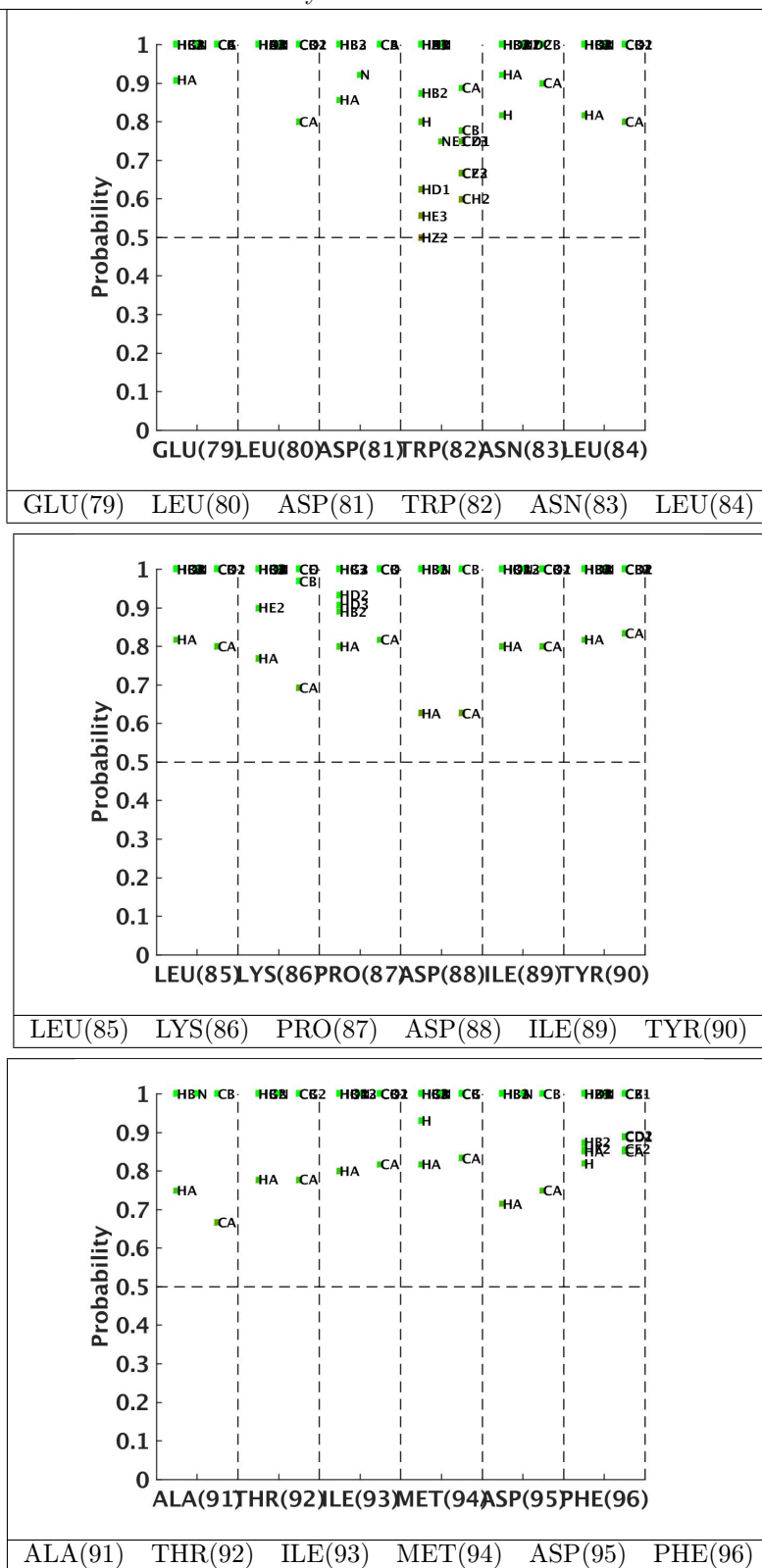


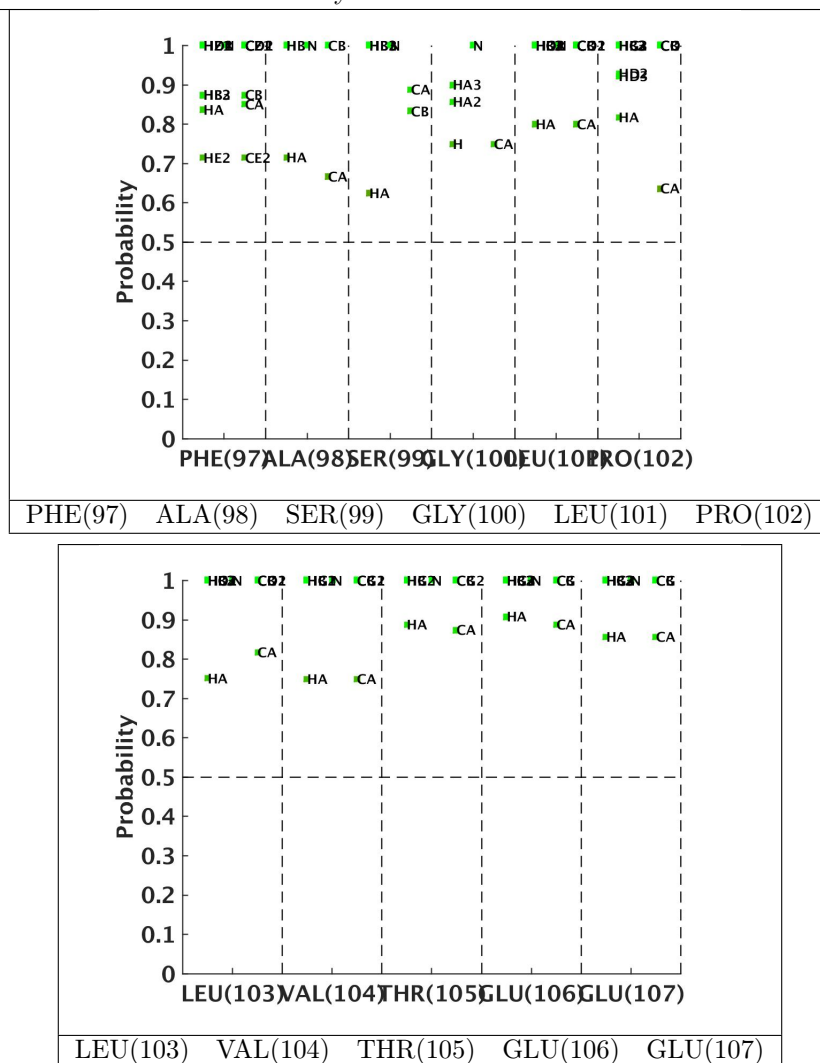












### 3 Residues Report

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)

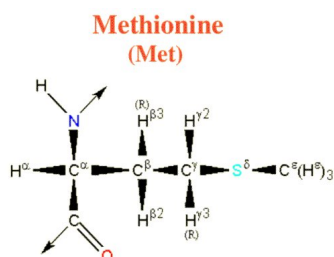


Figure 1: Image from the BMRB

Residue probability: 0.946

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	0.875	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	1.000	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	0.875	0.875
HB2 3.11.6	2.197	2.016	0.340	0.857	0.875
HB3 3.11.7	2.311	1.978	0.359	0.857	0.875
HG2 3.11.8	1.795	2.410	0.360	1.000	0.875
HG3 3.11.9	1.786	2.378	0.386	1.000	0.875
HE 3.11.10	1.791	1.877	0.381	1.000	1.000
H	NA	—	—	0.000	0.000

## 3.11.1 Detailed Probabilities of MET11CA:

Overall probability: 0.875

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
MET11	1.00	0.83
PHE12	0.50	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	0.000	1.00	0.00
MET11	HB2	1.00	0.001	1.00	0.00
MET11	HB3	1.00	0.005	1.00	0.00
MET11	HG2	1.00	0.016	1.00	0.00
MET11	HG3	1.00	0.007	1.00	0.00
MET11	HE1	0.69	0.012	1.00	0.00
PHE12	HA	1.00	0.386	0.00	0.00
PHE12	H	1.00	0.004	1.00	0.00

**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	0.006	1.00	0.00
MET11	HB2	1.00	0.000	1.00	0.00
MET11	HB3	1.00	0.008	1.00	0.00
MET11	HG2	1.00	0.006	1.00	0.00
MET11	HG3	1.00	0.003	1.00	0.00
MET11	HE1	0.96	0.002	1.00	0.00
PHE12	H	1.00	0.006	1.00	0.00

**3.11.3 Detailed Probabilities of MET11CG:**

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
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	0.000	1.00	0.00
MET11	HB2	1.00	0.004	1.00	0.00
MET11	HB3	1.00	0.005	1.00	0.00
MET11	HG2	1.00	0.000	1.00	0.00
MET11	HG3	1.00	0.009	1.00	0.00
MET11	HE1	1.00	0.004	1.00	0.00
PHE12	H	0.98	0.017	1.00	0.00

**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	0.006	1.00	0.00
MET11	HB3	0.97	0.010	1.00	0.00
MET11	HG2	1.00	0.004	1.00	0.00
MET11	HG3	1.00	0.005	1.00	0.00
MET11	HE1	1.00	0.000	1.00	0.00
MET11	HA	0.67	0.019	1.00	0.00

**3.11.5 Detailed Probabilities of MET11HA:**

Overall probability: 0.875

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
MET11	1.00	0.83
PHE12	0.50	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	0.000	1.00	0.00
MET11	HB2	1.00	0.006	1.00	0.00
MET11	HB3	1.00	0.000	1.00	0.00
MET11	HG2	1.00	0.000	1.00	0.00
MET11	HG3	1.00	0.000	1.00	0.00
MET11	HE1	0.69	0.019	1.00	0.00
PHE12	HA	1.00	0.362	0.00	0.00
PHE12	H	1.00	0.006	1.00	0.00

**3.11.6 Detailed Probabilities of MET11HB2:**

Overall probability: 0.857

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
MET11	1.00	0.86
PHE12	0.00	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	0.001	1.00	0.00
MET11	HB2	1.00	0.000	1.00	0.00
MET11	HB3	1.00	0.004	1.00	0.00
MET11	HG2	1.00	0.004	1.00	0.00
MET11	HG3	1.00	0.004	1.00	0.00
MET11	HE1	0.96	0.006	1.00	0.00
PHE12	H	1.00	0.401	0.00	0.00

**3.11.7 Detailed Probabilities of MET11HB3:**

Overall probability: 0.857

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
MET11	1.00	0.86
PHE12	0.00	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	0.00
MET11	HB2	1.00	0.008	1.00	0.00
MET11	HB3	1.00	0.000	1.00	0.00
MET11	HG2	1.00	0.005	1.00	0.00
MET11	HG3	1.00	0.005	1.00	0.00
MET11	HE1	0.97	0.010	1.00	0.00
PHE12	H	1.00	0.515	0.00	0.00

**3.11.8 Detailed Probabilities of MET11HG2:**

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
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	0.016	1.00	0.00
MET11	HB2	1.00	0.006	1.00	0.00
MET11	HB3	1.00	0.010	1.00	0.00
MET11	HG2	1.00	0.000	1.00	0.00
MET11	HG3	1.00	0.000	1.00	0.00
MET11	HE1	1.00	0.004	1.00	0.00
PHE12	H	0.98	0.001	1.00	0.00

**3.11.9 Detailed Probabilities of MET11HG3:**

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
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	0.007	1.00	0.00
MET11	HB2	1.00	0.003	1.00	0.00
MET11	HB3	1.00	0.001	1.00	0.00
MET11	HG2	1.00	0.009	1.00	0.00
MET11	HG3	1.00	0.009	1.00	0.00
MET11	HE1	1.00	0.005	1.00	0.00
PHE12	H	0.97	0.010	1.00	0.00

**3.11.10 Detailed Probabilities of MET11HE1:**

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	0.00
MET11	HB3	0.97	0.006	1.00	0.00
MET11	HG2	1.00	0.004	1.00	0.00
MET11	HG3	1.00	0.004	1.00	0.00
MET11	HE1	1.00	0.000	1.00	0.00
MET11	HA	0.67	0.012	1.00	0.00

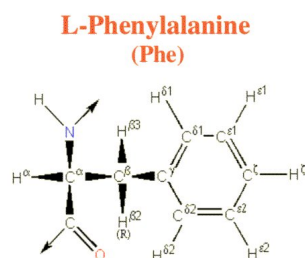
**3.12 PHE(12)**

Figure 2: Image from the BMRB

Residue probability: 0.881

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	0.700	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	0.889	1.000
CD2 3.12.4	131.845	131.352	9.581	0.891	1.000
CE1 3.12.5	131.421	130.599	3.219	1.000	1.000
CE2 3.12.6	131.667	130.633	2.839	0.857	1.000
CZ 3.12.7	129.788	129.042	3.448	1.000	1.000
N 3.12.8	121.868	120.315	4.931	0.773	0.929
HA 3.12.9	4.641	4.625	1.237	0.778	0.900
HB2 3.12.10	3.024	2.980	0.399	1.000	1.000
HB3 3.12.11	2.977	2.916	0.434	0.875	1.000
HD1 3.12.12	7.187	7.037	0.347	1.000	1.000
HD2 3.12.13	7.187	7.022	0.417	1.000	1.000
HE1 3.12.14	7.229	7.046	0.417	1.000	1.000
HE2 3.12.15	7.229	7.043	0.400	0.715	1.000
HZ 3.12.16	7.276	6.984	1.598	1.000	1.000
H 3.12.17	8.451	8.375	0.710	0.620	0.929

**3.12.1 Detailed Probabilities of PHE12CA:**

Overall probability: 0.700

Overall confidence: 0.900

**Inter- and intra-residue probability**

Residue	Probability	Confidence
MET11	0.00	0.50
PHE12	0.83	1.00
ILE13	0.67	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	0.362	0.00	0.00
PHE12	HA	1.00	0.000	1.00	0.00
PHE12	HB2	1.00	0.000	1.00	0.00
PHE12	HB3	1.00	0.000	1.00	0.00
PHE12	HD1	1.00	0.001	1.00	0.00
PHE12	HD2	1.00	0.001	1.00	0.00
PHE12	H	1.00	0.297	0.00	0.00
ILE13	HA	1.00	0.468	0.00	0.00
ILE13	H	1.00	0.000	1.00	0.00
ILE13	HG13	0.66	0.014	1.00	0.00

**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
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**

## 3.12 PHE(12)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE12	HA	1.00	0.000	1.00	0.00
PHE12	HB2	1.00	0.000	1.00	0.00
PHE12	HB3	1.00	0.000	1.00	0.00
PHE12	HD1	1.00	0.001	1.00	0.00
PHE12	HD2	1.00	0.001	1.00	0.00
PHE12	HE2	1.00	0.043	0.00	0.00
PHE12	H	1.00	0.002	1.00	0.00
ILE13	H	1.00	0.000	1.00	0.00

## 3.12.3 Detailed Probabilities of PHE12CD1:

Overall probability: 0.889

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
PHE12	0.89	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	0.000	1.00	0.00
PHE12	HB2	1.00	0.000	1.00	0.00
PHE12	HB3	1.00	0.000	1.00	0.00
PHE12	HD1	1.00	0.001	1.00	0.00
PHE12	HD2	1.00	0.001	1.00	0.00
PHE12	HE1	1.00	0.003	1.00	0.00
PHE12	HE2	1.00	0.003	1.00	0.00
PHE12	HZ	1.00	0.000	1.00	0.00
PHE12	H	1.00	0.565	0.00	0.00

## 3.12.4 Detailed Probabilities of PHE12CD2:

Overall probability: 0.891

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
PHE12	0.89	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	0.000	1.00	0.00
PHE12	HB2	1.00	0.000	1.00	0.00
PHE12	HB3	1.00	0.000	1.00	0.00
PHE12	HD1	1.00	0.001	1.00	0.00
PHE12	HD2	1.00	0.001	1.00	0.00
PHE12	HE1	1.00	0.003	1.00	0.00
PHE12	HE2	1.00	0.003	1.00	0.00
PHE12	HZ	1.00	0.000	1.00	0.00
PHE12	H	0.99	0.565	0.01	0.00

**3.12.5 Detailed Probabilities of PHE12CE1:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE12	1.00	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	0.001	1.00	0.00
PHE12	HD2	1.00	0.001	1.00	0.00
PHE12	HE1	1.00	0.003	1.00	0.00
PHE12	HE2	1.00	0.003	1.00	0.00
PHE12	HZ	1.00	0.000	1.00	0.00
PHE12	HB2	0.90	0.012	1.00	0.00

**3.12.6 Detailed Probabilities of PHE12CE2:**

Overall probability: 0.857

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE12	0.86	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	0.012	1.00	0.00
PHE12	HB3	1.00	0.184	0.00	0.00
PHE12	HD1	1.00	0.001	1.00	0.00
PHE12	HD2	1.00	0.001	1.00	0.00
PHE12	HE1	1.00	0.003	1.00	0.00
PHE12	HE2	1.00	0.003	1.00	0.00
PHE12	HZ	1.00	0.000	1.00	0.00

**3.12.7 Detailed Probabilities of PHE12CZ:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE12	1.00	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	0.001	1.00	0.00
PHE12	HD2	1.00	0.001	1.00	0.00
PHE12	HE1	1.00	0.003	1.00	0.00
PHE12	HE2	1.00	0.003	1.00	0.00
PHE12	HZ	1.00	0.000	1.00	0.00

**3.12.8 Detailed Probabilities of PHE12N:**

Overall probability: 0.773

Overall confidence: 0.929

**Inter- and intra-residue probability**

Residue	Probability	Confidence
MET11	0.60	0.83
PHE12	1.00	1.00
ILE13	0.52	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	0.006	1.00	0.00
MET11	HB2	1.00	0.401	0.00	0.00
MET11	HB3	1.00	0.515	0.00	0.00
MET11	HG2	0.98	0.001	1.00	0.00
MET11	HG3	0.97	0.010	1.00	0.00
PHE12	HA	1.00	0.008	1.00	0.00
PHE12	HB2	1.00	0.019	1.00	0.00
PHE12	HB3	1.00	0.028	1.00	0.00
PHE12	HD1	1.00	0.005	1.00	0.00
PHE12	HD2	0.99	0.005	1.00	0.00
PHE12	H	1.00	0.000	1.00	0.00
ILE13	HA	0.96	0.100	0.04	0.00
ILE13	H	1.00	0.007	1.00	0.00

**3.12.9 Detailed Probabilities of PHE12HA:**

Overall probability: 0.778

Overall confidence: 0.900

**Inter- and intra-residue probability**

Residue	Probability	Confidence
MET11	0.00	0.50
PHE12	1.00	1.00
ILE13	0.50	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	0.386	0.00	0.00
PHE12	HA	1.00	0.000	1.00	0.00
PHE12	HB2	1.00	0.000	1.00	0.00
PHE12	HB3	1.00	0.000	1.00	0.00
PHE12	HD1	1.00	0.000	1.00	0.00
PHE12	HD2	1.00	0.000	1.00	0.00
PHE12	H	1.00	0.008	1.00	0.00
ILE13	HA	1.00	0.117	0.00	0.00
ILE13	H	1.00	0.000	1.00	0.00

**3.12.10 Detailed Probabilities of PHE12HB2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE12	1.00	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	0.000	1.00	0.00
PHE12	HB2	1.00	0.000	1.00	0.00
PHE12	HB3	1.00	0.000	1.00	0.00
PHE12	HD1	1.00	0.000	1.00	0.00
PHE12	HD2	1.00	0.000	1.00	0.00
PHE12	HE2	1.00	0.012	1.00	0.00
PHE12	H	1.00	0.019	1.00	0.00
PHE12	HE1	0.90	0.012	1.00	0.00
ILE13	H	1.00	0.000	1.00	0.00

**3.12.11 Detailed Probabilities of PHE12HB3:**

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	0.000	1.00	0.00
PHE12	HB2	1.00	0.000	1.00	0.00
PHE12	HB3	1.00	0.000	1.00	0.00
PHE12	HD1	1.00	0.000	1.00	0.00
PHE12	HD2	1.00	0.000	1.00	0.00
PHE12	HE2	1.00	0.184	0.00	0.00
PHE12	H	1.00	0.028	1.00	0.00
ILE13	H	1.00	0.000	1.00	0.00

**3.12.12 Detailed Probabilities of PHE12HD1:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE12	1.00	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	0.001	1.00	0.00
PHE12	HB2	1.00	0.001	1.00	0.00
PHE12	HB3	1.00	0.001	1.00	0.00
PHE12	HD1	1.00	0.001	1.00	0.00
PHE12	HD2	1.00	0.001	1.00	0.00
PHE12	HE1	1.00	0.001	1.00	0.00
PHE12	HE2	1.00	0.001	1.00	0.00
PHE12	HZ	1.00	0.001	1.00	0.00
PHE12	H	1.00	0.005	1.00	0.00

**3.12.13 Detailed Probabilities of PHE12HD2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE12	1.00	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	0.001	1.00	0.00
PHE12	HB2	1.00	0.001	1.00	0.00
PHE12	HB3	1.00	0.001	1.00	0.00
PHE12	HD1	1.00	0.001	1.00	0.00
PHE12	HD2	1.00	0.001	1.00	0.00
PHE12	HE1	1.00	0.001	1.00	0.00
PHE12	HE2	1.00	0.001	1.00	0.00
PHE12	HZ	1.00	0.001	1.00	0.00
PHE12	H	0.99	0.005	1.00	0.00

**3.12.14 Detailed Probabilities of PHE12HE1:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE12	1.00	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	0.003	1.00	0.00
PHE12	HD2	1.00	0.003	1.00	0.00
PHE12	HE1	1.00	0.003	1.00	0.00
PHE12	HE2	1.00	0.003	1.00	0.00
PHE12	HZ	1.00	0.003	1.00	0.00

**3.12.15 Detailed Probabilities of PHE12HE2:**

Overall probability: 0.715

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE12	0.71	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	0.043	0.00	0.00
PHE12	HB3	1.00	0.043	0.00	0.00
PHE12	HD1	1.00	0.003	1.00	0.00
PHE12	HD2	1.00	0.003	1.00	0.00
PHE12	HE1	1.00	0.003	1.00	0.00
PHE12	HE2	1.00	0.003	1.00	0.00
PHE12	HZ	1.00	0.003	1.00	0.00

**3.12.16 Detailed Probabilities of PHE12HZ:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE12	1.00	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	0.000	1.00	0.00
PHE12	HD2	1.00	0.000	1.00	0.00
PHE12	HE1	1.00	0.000	1.00	0.00
PHE12	HE2	1.00	0.000	1.00	0.00
PHE12	HZ	1.00	0.000	1.00	0.00

**3.12.17 Detailed Probabilities of PHE12H:**

Overall probability: 0.620

Overall confidence: 0.929

**Inter- and intra-residue probability**

Residue	Probability	Confidence
MET11	1.00	0.83
PHE12	0.50	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	0.00
MET11	HB2	1.00	0.006	1.00	0.00
MET11	HB3	1.00	0.022	1.00	0.00
MET11	HG2	0.98	0.017	1.00	0.00
MET11	HG3	0.97	0.017	1.00	0.00
PHE12	HA	1.00	0.297	0.00	0.00
PHE12	HB2	1.00	0.002	1.00	0.00
PHE12	HB3	1.00	0.002	1.00	0.00
PHE12	HD1	1.00	0.565	0.00	0.00
PHE12	HD2	0.99	0.565	0.01	0.00
PHE12	H	1.00	0.000	1.00	0.00
ILE13	HA	0.96	0.501	0.04	0.00
ILE13	H	1.00	0.501	0.00	0.00

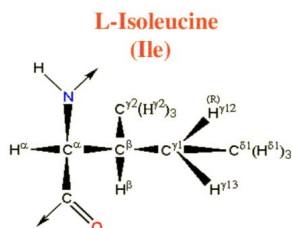


Figure 3: Image from the BMRB

Residue probability: 0.952  
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	0.917	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	1.000	1.000
HG12 3.13.9	1.491	1.271	0.411	1.000	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	1.000	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	0.117	0.00	0.00
PHE12	H	0.96	0.501	0.04	0.00
ILE13	HA	1.00	0.000	1.00	0.00
ILE13	HB	1.00	0.000	1.00	0.00
ILE13	HG12	1.00	0.000	1.00	0.00
ILE13	HG13	1.00	0.000	1.00	0.00
ILE13	HG21	1.00	0.000	1.00	0.00
ILE13	HD11	0.97	0.000	1.00	0.00
ILE13	H	1.00	0.000	1.00	0.00
GLN14	HA	1.00	0.063	0.00	0.00
GLN14	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ILE13	HB	1.00	0.000	1.00	0.00
ILE13	HG12	1.00	0.000	1.00	0.00
ILE13	HG13	1.00	0.000	1.00	0.00
ILE13	HG21	1.00	0.000	1.00	0.00
ILE13	HD11	1.00	0.000	1.00	0.00
ILE13	H	1.00	0.000	1.00	0.00
GLN14	H	1.00	0.000	1.00	0.00

#### 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
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	0.000	1.00	0.00
ILE13	HB	1.00	0.000	1.00	0.00
ILE13	HG12	1.00	0.000	1.00	0.00
ILE13	HG13	1.00	0.000	1.00	0.00
ILE13	HG21	1.00	0.000	1.00	0.00
ILE13	HD11	1.00	0.000	1.00	0.00
ILE13	H	1.00	0.000	1.00	0.00
GLN14	H	0.99	0.000	1.00	0.00

#### 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	0.000	1.00	0.00
ILE13	HB	1.00	0.000	1.00	0.00
ILE13	HG12	1.00	0.000	1.00	0.00
ILE13	HG13	1.00	0.000	1.00	0.00
ILE13	HG21	1.00	0.000	1.00	0.00
ILE13	HD11	0.99	0.000	1.00	0.00
ILE13	H	1.00	0.000	1.00	0.00
GLN14	H	0.99	0.000	1.00	0.00

**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	0.000	1.00	0.00
ILE13	HB	1.00	0.000	1.00	0.00
ILE13	HG12	1.00	0.000	1.00	0.00
ILE13	HG13	1.00	0.000	1.00	0.00
ILE13	HG21	0.99	0.000	1.00	0.00
ILE13	HD11	1.00	0.000	1.00	0.00
ILE13	H	0.94	0.000	1.00	0.00

**3.13.6 Detailed Probabilities of ILE13N:**

Overall probability: 0.917

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	0.000	1.00	0.00
PHE12	HB2	1.00	0.000	1.00	0.00
PHE12	HB3	1.00	0.000	1.00	0.00
PHE12	H	1.00	0.501	0.00	0.00
ILE13	HA	1.00	0.000	1.00	0.00
ILE13	HB	1.00	0.000	1.00	0.00
ILE13	HG12	1.00	0.000	1.00	0.00
ILE13	HG13	1.00	0.000	1.00	0.00
ILE13	HG21	1.00	0.000	1.00	0.00
ILE13	H	1.00	0.000	1.00	0.00
ILE13	HD11	0.94	0.000	1.00	0.00
GLN14	H	1.00	0.025	1.00	0.00

**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	0.468	0.00	0.00
PHE12	H	0.96	0.100	0.04	0.00
ILE13	HA	1.00	0.000	1.00	0.00
ILE13	HB	1.00	0.000	1.00	0.00
ILE13	HG12	1.00	0.000	1.00	0.00
ILE13	HG13	1.00	0.000	1.00	0.00
ILE13	HG21	1.00	0.000	1.00	0.00
ILE13	HD11	0.97	0.000	1.00	0.00
ILE13	H	1.00	0.000	1.00	0.00
GLN14	HA	1.00	0.438	0.00	0.00
GLN14	H	1.00	0.000	1.00	0.00

**3.13.8 Detailed Probabilities of ILE13HB:**

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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE13	HA	1.00	0.000	1.00	0.00
ILE13	HB	1.00	0.000	1.00	0.00
ILE13	HG12	1.00	0.000	1.00	0.00
ILE13	HG13	1.00	0.000	1.00	0.00
ILE13	HG21	1.00	0.000	1.00	0.00
ILE13	HD11	1.00	0.000	1.00	0.00
ILE13	H	1.00	0.000	1.00	0.00
GLN14	H	1.00	0.000	1.00	0.00

**3.13.9 Detailed Probabilities of ILE13HG12:**

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
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	0.000	1.00	0.00
ILE13	HB	1.00	0.000	1.00	0.00
ILE13	HG12	1.00	0.000	1.00	0.00
ILE13	HG13	1.00	0.000	1.00	0.00
ILE13	HG21	1.00	0.000	1.00	0.00
ILE13	HD11	1.00	0.000	1.00	0.00
ILE13	H	1.00	0.000	1.00	0.00
GLN14	H	0.99	0.000	1.00	0.00

**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	0.000	1.00	0.00
ILE13	HB	1.00	0.000	1.00	0.00
ILE13	HG12	1.00	0.000	1.00	0.00
ILE13	HG13	1.00	0.000	1.00	0.00
ILE13	HG21	1.00	0.000	1.00	0.00
ILE13	HD11	1.00	0.000	1.00	0.00
ILE13	H	1.00	0.000	1.00	0.00

**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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE13	HA	1.00	0.000	1.00	0.00
ILE13	HB	1.00	0.000	1.00	0.00
ILE13	HG12	1.00	0.000	1.00	0.00
ILE13	HG13	1.00	0.000	1.00	0.00
ILE13	HG21	1.00	0.000	1.00	0.00
ILE13	HD11	0.99	0.000	1.00	0.00
ILE13	H	1.00	0.000	1.00	0.00
GLN14	H	0.99	0.000	1.00	0.00
GLN14	HA	0.69	0.001	1.00	0.00

**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	0.000	1.00	0.00
ILE13	HB	1.00	0.000	1.00	0.00
ILE13	HG12	1.00	0.000	1.00	0.00
ILE13	HG13	1.00	0.000	1.00	0.00
ILE13	HG21	0.99	0.000	1.00	0.00
ILE13	HD11	1.00	0.000	1.00	0.00
ILE13	H	0.94	0.000	1.00	0.00

**3.13.13 Detailed Probabilities of ILE13H:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE12	1.00	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	0.000	1.00	0.00
PHE12	HB2	1.00	0.000	1.00	0.00
PHE12	HB3	1.00	0.000	1.00	0.00
PHE12	H	1.00	0.007	1.00	0.00
ILE13	HA	1.00	0.000	1.00	0.00
ILE13	HB	1.00	0.000	1.00	0.00
ILE13	HG12	1.00	0.000	1.00	0.00
ILE13	HG13	1.00	0.000	1.00	0.00
ILE13	HG21	1.00	0.000	1.00	0.00
ILE13	H	1.00	0.000	1.00	0.00
ILE13	HD11	0.94	0.000	1.00	0.00
GLN14	H	1.00	0.025	1.00	0.00
GLN14	HA	0.93	0.025	1.00	0.00
GLN14	HB2	0.56	0.025	1.00	0.00

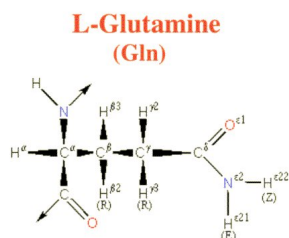


Figure 4: Image from the BMRB

Residue probability: 0.905  
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	0.818	1.000
CB 3.14.2	31.276	29.436	2.799	0.889	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	0.778	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	0.889	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	1.000	1.000
H 3.14.11	7.925	8.232	0.711	1.000	1.000
HE21 3.14.12	7.513	7.217	0.496	0.833	1.000
HE22 3.14.13	6.854	7.041	0.463	0.667	1.000

**3.14.1 Detailed Probabilities of GLN14CA:**

Overall probability: 0.818  
Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE13	0.67	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	0.438	0.00	0.00
ILE13	HG21	0.70	0.001	1.00	0.00
ILE13	H	0.93	0.025	1.00	0.00
GLN14	HA	1.00	0.000	1.00	0.00
GLN14	HB2	1.00	0.000	1.00	0.00
GLN14	HB3	1.00	0.000	1.00	0.00
GLN14	HG2	1.00	0.000	1.00	0.00
GLN14	HG3	1.00	0.000	1.00	0.00
GLN14	H	1.00	0.000	1.00	0.00
THR15	HA	1.00	0.638	0.00	0.00
THR15	H	1.00	0.000	1.00	0.00

**3.14.2 Detailed Probabilities of GLN14CB:**

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**

## 3.14 GLN(14)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN14	HA	1.00	0.000	1.00	0.00
GLN14	HB2	1.00	0.000	1.00	0.00
GLN14	HB3	1.00	0.000	1.00	0.00
GLN14	HG2	1.00	0.000	1.00	0.00
GLN14	HG3	1.00	0.000	1.00	0.00
GLN14	H	1.00	0.000	1.00	0.00
GLN14	HE21	1.00	0.026	1.00	0.00
GLN14	HE22	1.00	0.338	0.00	0.00
THR15	H	1.00	0.000	1.00	0.00

## 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
Q14HG3	1.00
Q14H	1.00
Q14HE21	1.00
Q14HE22	1.00
Q14HG2	1.00
T15H	0.97

## NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN14	HA	1.00	0.000	1.00	0.00
GLN14	HB2	1.00	0.000	1.00	0.00
GLN14	HB3	1.00	0.000	1.00	0.00
GLN14	HG2	1.00	0.000	1.00	0.00
GLN14	HG3	1.00	0.000	1.00	0.00
GLN14	H	1.00	0.000	1.00	0.00
GLN14	HE21	1.00	0.000	1.00	0.00
GLN14	HE22	1.00	0.000	1.00	0.00
THR15	H	0.97	0.000	1.00	0.00

## 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	0.000	1.00	0.00
ILE13	HB	1.00	0.000	1.00	0.00
ILE13	HG12	0.99	0.000	1.00	0.00
ILE13	HG21	0.99	0.000	1.00	0.00
ILE13	H	1.00	0.025	1.00	0.00
ILE13	HG13	0.94	0.000	1.00	0.00
GLN14	HA	1.00	0.000	1.00	0.00
GLN14	HB2	1.00	0.000	1.00	0.00
GLN14	HB3	1.00	0.000	1.00	0.00
GLN14	HG2	1.00	0.000	1.00	0.00
GLN14	HG3	1.00	0.000	1.00	0.00
GLN14	H	1.00	0.000	1.00	0.00
THR15	H	1.00	0.000	1.00	0.00

**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	0.001	1.00	0.00
GLN14	HB3	1.00	0.004	1.00	0.00
GLN14	HG2	1.00	0.000	1.00	0.00
GLN14	HG3	1.00	0.000	1.00	0.00
GLN14	HE21	1.00	0.000	1.00	0.00
GLN14	HE22	1.00	0.000	1.00	0.00

**3.14.6 Detailed Probabilities of GLN14HA:**

Overall probability: 0.778

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	0.000	1.00	0.00
GLN14	HB2	1.00	0.000	1.00	0.00
GLN14	HB3	1.00	0.000	1.00	0.00
GLN14	HG2	1.00	0.000	1.00	0.00
GLN14	HG3	1.00	0.000	1.00	0.00
GLN14	H	1.00	0.000	1.00	0.00
THR15	HA	1.00	0.638	0.00	0.00
THR15	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
GLN14	HB2	1.00	0.000	1.00	0.00
GLN14	HB3	1.00	0.000	1.00	0.00
GLN14	HG2	1.00	0.000	1.00	0.00
GLN14	HG3	1.00	0.000	1.00	0.00
GLN14	H	1.00	0.000	1.00	0.00
GLN14	HE21	1.00	0.001	1.00	0.00
GLN14	HE22	1.00	0.127	0.00	0.00
THR15	H	1.00	0.000	1.00	0.00

**3.14.8 Detailed Probabilities of GLN14HB3:**

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
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	0.000	1.00	0.00
GLN14	HB2	1.00	0.000	1.00	0.00
GLN14	HB3	1.00	0.000	1.00	0.00
GLN14	HG2	1.00	0.000	1.00	0.00
GLN14	HG3	1.00	0.000	1.00	0.00
GLN14	H	1.00	0.000	1.00	0.00
GLN14	HE21	1.00	0.004	1.00	0.00
GLN14	HE22	1.00	0.350	0.00	0.00
THR15	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
GLN14	HB2	1.00	0.000	1.00	0.00
GLN14	HB3	1.00	0.000	1.00	0.00
GLN14	HG2	1.00	0.000	1.00	0.00
GLN14	HG3	1.00	0.000	1.00	0.00
GLN14	H	1.00	0.000	1.00	0.00
GLN14	HE21	1.00	0.000	1.00	0.00
GLN14	HE22	1.00	0.000	1.00	0.00
THR15	H	0.97	0.000	1.00	0.00

## 3.14.10 Detailed Probabilities of GLN14HG3:

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	0.000	1.00	0.00
GLN14	HB2	1.00	0.000	1.00	0.00
GLN14	HB3	1.00	0.000	1.00	0.00
GLN14	HG2	1.00	0.000	1.00	0.00
GLN14	HG3	1.00	0.000	1.00	0.00
GLN14	H	1.00	0.000	1.00	0.00
GLN14	HE21	1.00	0.000	1.00	0.00
GLN14	HE22	1.00	0.000	1.00	0.00
THR15	H	0.95	0.000	1.00	0.00

## 3.14.11 Detailed Probabilities of GLN14H:

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	0.000	1.00	0.00
ILE13	HB	1.00	0.000	1.00	0.00
ILE13	HG12	0.99	0.000	1.00	0.00
ILE13	HG21	0.99	0.000	1.00	0.00
ILE13	H	1.00	0.025	1.00	0.00
ILE13	HG13	0.94	0.000	1.00	0.00
GLN14	HA	1.00	0.000	1.00	0.00
GLN14	HB2	1.00	0.000	1.00	0.00
GLN14	HB3	1.00	0.000	1.00	0.00
GLN14	HG2	1.00	0.000	1.00	0.00
GLN14	HG3	1.00	0.000	1.00	0.00
GLN14	H	1.00	0.000	1.00	0.00
THR15	H	1.00	0.000	1.00	0.00

**3.14.12 Detailed Probabilities of GLN14HE21:**

Overall probability: 0.833

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLN14	0.83	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	0.026	1.00	0.00
GLN14	HB3	1.00	0.412	0.00	0.00
GLN14	HG2	1.00	0.000	1.00	0.00
GLN14	HG3	1.00	0.000	1.00	0.00
GLN14	HE21	1.00	0.000	1.00	0.00
GLN14	HE22	1.00	0.000	1.00	0.00

**3.14.13 Detailed Probabilities of GLN14HE22:**

Overall probability: 0.667

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLN14	0.67	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	0.338	0.00	0.00
GLN14	HB3	1.00	0.186	0.00	0.00
GLN14	HG2	1.00	0.000	1.00	0.00
GLN14	HG3	1.00	0.000	1.00	0.00
GLN14	HE21	1.00	0.000	1.00	0.00
GLN14	HE22	1.00	0.000	1.00	0.00

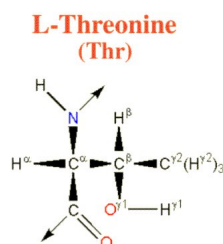
**3.15 THR(15)**

Figure 5: Image from the BMRB

Residue probability: 0.907

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	0.917	0.917
HA 3.15.5	5.225	4.461	0.626	0.714	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	0.909	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	0.638	0.00	0.00
THR15	HA	1.00	0.000	1.00	0.00
THR15	HB	1.00	0.000	1.00	0.00
THR15	HG21	1.00	0.000	1.00	0.00
THR15	H	1.00	0.000	1.00	0.00
GLN16	HA	1.00	0.742	0.00	0.00
GLN16	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
THR15	HB	1.00	0.000	1.00	0.00
THR15	HG21	1.00	0.000	1.00	0.00
THR15	H	1.00	0.000	1.00	0.00
GLN16	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
THR15	HB	1.00	0.000	1.00	0.00
THR15	HG21	1.00	0.000	1.00	0.00
THR15	H	1.00	0.000	1.00	0.00
GLN16	H	0.96	0.000	1.00	0.00

**3.15.4 Detailed Probabilities of THR15N:**

Overall probability: 0.917

Overall confidence: 0.917

**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
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)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN14	HA	1.00	0.000	1.00	0.00
GLN14	HB2	1.00	0.000	1.00	0.00
GLN14	HB3	1.00	0.000	1.00	0.00
GLN14	HG2	0.97	0.000	1.00	0.00
GLN14	HG3	0.95	0.000	1.00	0.00
GLN14	H	1.00	0.000	1.00	0.00
THR15	HA	1.00	0.000	1.00	0.00
THR15	HB	1.00	0.000	1.00	0.00
THR15	HG21	1.00	0.000	1.00	0.00
THR15	H	1.00	0.000	1.00	0.00
GLN16	H	1.00	0.303	0.00	0.00
GLN16	HB2	0.56	0.024	1.00	0.00

## 3.15.5 Detailed Probabilities of THR15HA:

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	0.638	0.00	0.00
THR15	HA	1.00	0.000	1.00	0.00
THR15	HB	1.00	0.000	1.00	0.00
THR15	HG21	1.00	0.000	1.00	0.00
THR15	H	1.00	0.000	1.00	0.00
GLN16	HA	1.00	0.742	0.00	0.00
GLN16	H	1.00	0.000	1.00	0.00

## 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	0.000	1.00	0.00
THR15	HB	1.00	0.000	1.00	0.00
THR15	HG21	1.00	0.000	1.00	0.00
THR15	H	1.00	0.000	1.00	0.00
GLN16	H	1.00	0.000	1.00	0.00

**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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR15	HA	1.00	0.000	1.00	0.00
THR15	HB	1.00	0.000	1.00	0.00
THR15	HG21	1.00	0.000	1.00	0.00
THR15	H	1.00	0.000	1.00	0.00
GLN16	H	0.96	0.000	1.00	0.00

**3.15.8 Detailed Probabilities of THR15H:**

Overall probability: 0.909

Overall confidence: 0.917

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLN14	1.00	1.00
THR15	1.00	0.80
GLN16	0.00	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	0.000	1.00	0.00
GLN14	HB2	1.00	0.000	1.00	0.00
GLN14	HB3	1.00	0.000	1.00	0.00
GLN14	HG2	0.97	0.000	1.00	0.00
GLN14	HG3	0.95	0.000	1.00	0.00
GLN14	H	1.00	0.000	1.00	0.00
THR15	HA	1.00	0.000	1.00	0.00
THR15	HB	1.00	0.000	1.00	0.00
THR15	HG21	1.00	0.000	1.00	0.00
THR15	H	1.00	0.000	1.00	0.00
GLN16	H	1.00	0.176	0.00	0.00

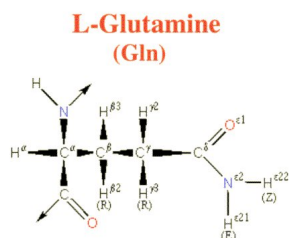
**3.16 GLN(16)**

Figure 6: Image from the BMRB

Residue probability: 0.823

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	0.778	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	0.889	1.000
N 3.16.4	121.949	119.799	3.762	0.909	0.917
NE2 3.16.5	111.338	111.924	2.434	0.833	1.000
HA 3.16.6	4.483	4.265	0.455	0.778	1.000
HB2 3.16.7	1.902	2.047	0.290	0.778	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	1.000	1.000
H 3.16.11	8.776	8.232	0.711	0.727	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: 0.778

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR15	0.00	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	0.742	0.00	0.00
GLN16	HA	1.00	0.000	1.00	0.00
GLN16	HB2	1.00	0.000	1.00	0.00
GLN16	HB3	1.00	0.000	1.00	0.00
GLN16	HG2	1.00	0.000	1.00	0.00
GLN16	HG3	1.00	0.000	1.00	0.00
GLN16	H	1.00	0.000	1.00	0.00
ASP17	HA	1.00	0.134	0.00	0.00
ASP17	H	1.00	0.000	1.00	0.00

**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)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN16	HA	1.00	0.000	1.00	0.00
GLN16	HB2	1.00	0.000	1.00	0.00
GLN16	HB3	1.00	0.000	1.00	0.00
GLN16	HG2	1.00	0.000	1.00	0.00
GLN16	HG3	1.00	0.000	1.00	0.00
GLN16	H	1.00	0.000	1.00	0.00
GLN16	HE21	1.00	0.815	0.00	0.00
GLN16	HE22	1.00	1.493	0.00	0.00
ASP17	H	1.00	0.000	1.00	0.00

## 3.16.3 Detailed Probabilities of GLN16CG:

Overall probability: 0.889

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
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	0.000	1.00	0.00
GLN16	HB2	1.00	0.000	1.00	0.00
GLN16	HB3	1.00	0.000	1.00	0.00
GLN16	HG2	1.00	0.000	1.00	0.00
GLN16	HG3	1.00	0.000	1.00	0.00
GLN16	H	1.00	0.479	0.00	0.00
GLN16	HE21	1.00	0.000	1.00	0.00
GLN16	HE22	1.00	0.000	1.00	0.00
ASP17	H	0.98	0.000	1.00	0.00

## 3.16.4 Detailed Probabilities of GLN16N:

Overall probability: 0.909

Overall confidence: 0.917

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR15	0.75	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	0.000	1.00	0.00
THR15	HB	1.00	0.000	1.00	0.00
THR15	HG21	0.97	0.000	1.00	0.00
THR15	H	1.00	0.176	0.00	0.00
GLN16	HA	1.00	0.000	1.00	0.00
GLN16	HB2	1.00	0.000	1.00	0.00
GLN16	HB3	1.00	0.000	1.00	0.00
GLN16	HG2	1.00	0.000	1.00	0.00
GLN16	HG3	1.00	0.000	1.00	0.00
GLN16	H	1.00	0.000	1.00	0.00
ASP17	H	1.00	0.000	1.00	0.00

**3.16.5 Detailed Probabilities of GLN16NE2:**

Overall probability: 0.833

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLN16	0.83	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	0.229	0.00	0.00
GLN16	HB3	1.00	0.001	1.00	0.00
GLN16	HG2	1.00	0.000	1.00	0.00
GLN16	HG3	1.00	0.000	1.00	0.00
GLN16	HE21	1.00	0.000	1.00	0.00
GLN16	HE22	1.00	0.000	1.00	0.00

**3.16.6 Detailed Probabilities of GLN16HA:**

Overall probability: 0.778

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR15	0.00	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	0.742	0.00	0.00
GLN16	HA	1.00	0.000	1.00	0.00
GLN16	HB2	1.00	0.000	1.00	0.00
GLN16	HB3	1.00	0.000	1.00	0.00
GLN16	HG2	1.00	0.000	1.00	0.00
GLN16	HG3	1.00	0.000	1.00	0.00
GLN16	H	1.00	0.000	1.00	0.00
ASP17	HA	1.00	0.134	0.00	0.00
ASP17	H	1.00	0.000	1.00	0.00

**3.16.7 Detailed Probabilities of GLN16HB2:**

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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN16	HA	1.00	0.000	1.00	0.00
GLN16	HB2	1.00	0.000	1.00	0.00
GLN16	HB3	1.00	0.000	1.00	0.00
GLN16	HG2	1.00	0.000	1.00	0.00
GLN16	HG3	1.00	0.000	1.00	0.00
GLN16	H	1.00	0.000	1.00	0.00
GLN16	HE21	1.00	0.229	0.00	0.00
GLN16	HE22	1.00	0.336	0.00	0.00
ASP17	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
GLN16	HB2	1.00	0.000	1.00	0.00
GLN16	HB3	1.00	0.000	1.00	0.00
GLN16	HG2	1.00	0.000	1.00	0.00
GLN16	HG3	1.00	0.000	1.00	0.00
GLN16	H	1.00	0.000	1.00	0.00
GLN16	HE21	1.00	0.001	1.00	0.00
GLN16	HE22	1.00	0.564	0.00	0.00
ASP17	H	1.00	0.000	1.00	0.00
ASP17	HA	0.79	0.026	1.00	0.00

**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	0.000	1.00	0.00
GLN16	HB2	1.00	0.000	1.00	0.00
GLN16	HB3	1.00	0.000	1.00	0.00
GLN16	HG2	1.00	0.000	1.00	0.00
GLN16	HG3	1.00	0.000	1.00	0.00
GLN16	H	1.00	0.000	1.00	0.00
GLN16	HE21	1.00	0.000	1.00	0.00
GLN16	HE22	1.00	0.000	1.00	0.00
ASP17	H	0.98	0.000	1.00	0.00

**3.16.10 Detailed Probabilities of GLN16HG3:**

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
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	0.000	1.00	0.00
GLN16	HB2	1.00	0.000	1.00	0.00
GLN16	HB3	1.00	0.000	1.00	0.00
GLN16	HG2	1.00	0.000	1.00	0.00
GLN16	HG3	1.00	0.000	1.00	0.00
GLN16	H	1.00	0.000	1.00	0.00
GLN16	HE21	1.00	0.000	1.00	0.00
GLN16	HE22	1.00	0.000	1.00	0.00
ASP17	H	0.96	0.000	1.00	0.00

**3.16.11 Detailed Probabilities of GLN16H:**

Overall probability: 0.727

Overall confidence: 0.917

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR15	0.75	0.80
GLN16	0.67	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	0.000	1.00	0.00
THR15	HB	1.00	0.000	1.00	0.00
THR15	HG21	0.97	0.000	1.00	0.00
THR15	H	1.00	0.303	0.00	0.00
GLN16	HA	1.00	0.000	1.00	0.00
GLN16	HB2	1.00	0.000	1.00	0.00
GLN16	HB3	1.00	0.000	1.00	0.00
GLN16	HG2	1.00	0.479	0.00	0.00
GLN16	HG3	1.00	0.479	0.00	0.00
GLN16	H	1.00	0.000	1.00	0.00
ASP17	H	1.00	0.000	1.00	0.00

**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	0.815	0.00	0.00
GLN16	HB3	1.00	0.815	0.00	0.00
GLN16	HG2	1.00	0.000	1.00	0.00
GLN16	HG3	1.00	0.000	1.00	0.00
GLN16	HE21	1.00	0.000	1.00	0.00
GLN16	HE22	1.00	0.000	1.00	0.00

## 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	1.493	0.00	0.00
GLN16	HB3	1.00	1.493	0.00	0.00
GLN16	HG2	1.00	0.000	1.00	0.00
GLN16	HG3	1.00	0.000	1.00	0.00
GLN16	HE21	1.00	0.000	1.00	0.00
GLN16	HE22	1.00	0.000	1.00	0.00

**3.17 ASP(17)**

Figure 7: Image from the BMRB

Residue probability: 0.926

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	0.767	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	1.000	1.000
HD2	NA	—	—	0.000	0.000
HA 3.17.4	4.617	4.587	0.329	0.714	0.875
HB2 3.17.5	2.680	2.708	0.282	1.000	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: 0.767

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLN16	0.63	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	0.134	0.00	0.00
GLN16	HB3	0.79	0.026	1.00	0.00
GLN16	H	0.86	0.031	0.90	0.00
ASP17	HA	1.00	0.000	1.00	0.00
ASP17	HB2	1.00	0.000	1.00	0.00
ASP17	HB3	1.00	0.000	1.00	0.00
ASP17	H	1.00	0.000	1.00	0.00
THR18	HA	1.00	0.303	0.00	0.00
THR18	H	1.00	0.000	1.00	0.00

**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
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	0.000	1.00	0.00
ASP17	HB2	1.00	0.000	1.00	0.00
ASP17	HB3	1.00	0.000	1.00	0.00
ASP17	H	1.00	0.000	1.00	0.00
THR18	H	1.00	0.000	1.00	0.00

**3.17.3 Detailed Probabilities of ASP17N:**

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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN16	HA	1.00	0.000	1.00	0.00
GLN16	HB2	1.00	0.000	1.00	0.00
GLN16	HB3	1.00	0.000	1.00	0.00
GLN16	HG2	0.98	0.000	1.00	0.00
GLN16	HG3	0.96	0.000	1.00	0.00
GLN16	H	1.00	0.000	1.00	0.00
ASP17	HA	1.00	0.000	1.00	0.00
ASP17	HB2	1.00	0.000	1.00	0.00
ASP17	HB3	1.00	0.000	1.00	0.00
ASP17	H	1.00	0.000	1.00	0.00
THR18	H	1.00	0.000	1.00	0.00

**3.17.4 Detailed Probabilities of ASP17HA:**

Overall probability: 0.714

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLN16	0.00	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	0.134	0.00	0.00
ASP17	HA	1.00	0.000	1.00	0.00
ASP17	HB2	1.00	0.000	1.00	0.00
ASP17	HB3	1.00	0.000	1.00	0.00
ASP17	H	1.00	0.000	1.00	0.00
THR18	HA	1.00	0.109	0.00	0.00
THR18	H	1.00	0.000	1.00	0.00

**3.17.5 Detailed Probabilities of ASP17HB2:**

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
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	0.000	1.00	0.00
ASP17	HB2	1.00	0.000	1.00	0.00
ASP17	HB3	1.00	0.000	1.00	0.00
ASP17	H	1.00	0.000	1.00	0.00
THR18	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ASP17	HB2	1.00	0.000	1.00	0.00
ASP17	HB3	1.00	0.000	1.00	0.00
ASP17	H	1.00	0.000	1.00	0.00
THR18	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
GLN16	HB2	1.00	0.000	1.00	0.00
GLN16	HB3	1.00	0.000	1.00	0.00
GLN16	HG2	0.98	0.000	1.00	0.00
GLN16	HG3	0.96	0.000	1.00	0.00
GLN16	H	1.00	0.000	1.00	0.00
ASP17	HA	1.00	0.000	1.00	0.00
ASP17	HB2	1.00	0.000	1.00	0.00
ASP17	HB3	1.00	0.000	1.00	0.00
ASP17	H	1.00	0.000	1.00	0.00
THR18	H	1.00	0.000	1.00	0.00

## 3.18 THR(18)

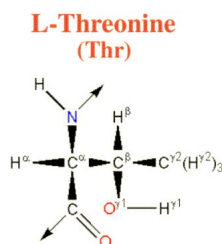


Figure 8: Image from the BMRB

Residue probability: 0.898

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	0.672	0.900
CB 3.18.2	69.312	69.395	4.500	1.000	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	0.900	0.900
HB 3.18.6	4.508	4.172	0.855	1.000	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	0.811	0.909
HG1	NA	—	—	0.000	0.000

## 3.18.1 Detailed Probabilities of THR18CA:

Overall probability: 0.672

Overall confidence: 0.900

## Inter- and intra-residue probability

Residue	Probability	Confidence
ASP17	0.00	1.00
THR18	1.00	0.80
PRO19	0.51	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	0.109	0.00	0.00
THR18	HA	1.00	0.000	1.00	0.00
THR18	HB	1.00	0.000	1.00	0.00
THR18	HG21	1.00	0.000	1.00	0.00
THR18	H	1.00	0.000	1.00	0.00
PRO19	HA	1.00	0.112	0.00	0.00
PRO19	HG2	0.95	0.063	0.05	0.00
PRO19	HD2	1.00	0.007	1.00	0.00
PRO19	HD3	1.00	0.006	1.00	0.00

**3.18.2 Detailed Probabilities of THR18CB:**

Overall probability: 1.000

Overall confidence: 0.857

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR18	1.00	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	0.00
THR18	HB	1.00	0.000	1.00	0.00
THR18	HG21	1.00	0.000	1.00	0.00
THR18	H	1.00	0.000	1.00	0.00
PRO19	HD2	0.99	0.005	1.00	0.00
PRO19	HD3	0.99	0.010	1.00	0.00

**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	0.000	1.00	0.00
THR18	HB	1.00	0.000	1.00	0.00
THR18	HG21	1.00	0.000	1.00	0.00
THR18	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ASP17	HB2	1.00	0.000	1.00	0.00
ASP17	HB3	1.00	0.000	1.00	0.00
ASP17	H	1.00	0.000	1.00	0.00
THR18	HA	1.00	0.000	1.00	0.00
THR18	HB	1.00	0.000	1.00	0.00
THR18	HG21	1.00	0.000	1.00	0.00
THR18	H	1.00	0.000	1.00	0.00
PRO19	HD2	1.00	0.663	0.00	0.00
PRO19	HD3	0.99	0.892	0.01	0.00

**3.18.5 Detailed Probabilities of THR18HA:**

Overall probability: 0.900

Overall confidence: 0.900

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASP17	0.00	1.00
THR18	1.00	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	0.303	0.00	0.00
THR18	HA	1.00	0.000	1.00	0.00
THR18	HB	1.00	0.000	1.00	0.00
THR18	HG21	1.00	0.000	1.00	0.00
THR18	H	1.00	0.000	1.00	0.00
PRO19	HA	1.00	0.019	1.00	0.00
PRO19	HG2	0.95	0.001	1.00	0.00
PRO19	HD2	1.00	0.005	1.00	0.00
PRO19	HD3	1.00	0.001	1.00	0.00
PRO19	HG3	0.94	0.001	1.00	0.00

**3.18.6 Detailed Probabilities of THR18HB:**

Overall probability: 1.000

Overall confidence: 0.857

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR18	1.00	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	0.00
THR18	HB	1.00	0.000	1.00	0.00
THR18	HG21	1.00	0.000	1.00	0.00
THR18	H	1.00	0.000	1.00	0.00
PRO19	HD2	0.99	0.003	1.00	0.00
PRO19	HD3	0.99	0.003	1.00	0.00

**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	0.000	1.00	0.00
THR18	HB	1.00	0.000	1.00	0.00
THR18	HG21	1.00	0.000	1.00	0.00
THR18	H	1.00	0.000	1.00	0.00

**3.18.8 Detailed Probabilities of THR18H:**

Overall probability: 0.811

Overall confidence: 0.909

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASP17	1.00	1.00
THR18	1.00	0.80
PRO19	0.05	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	0.000	1.00	0.00
ASP17	HB2	1.00	0.000	1.00	0.00
ASP17	HB3	1.00	0.000	1.00	0.00
ASP17	H	1.00	0.000	1.00	0.00
THR18	HA	1.00	0.000	1.00	0.00
THR18	HB	1.00	0.000	1.00	0.00
THR18	HG21	1.00	0.000	1.00	0.00
THR18	H	1.00	0.000	1.00	0.00
PRO19	HD2	1.00	0.039	0.10	0.00
PRO19	HD3	0.99	0.914	0.01	0.00

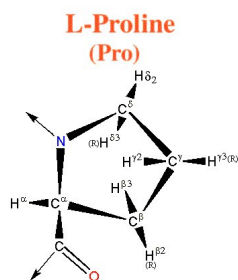


Figure 9: Image from the BMRB

**Residue probability:** 0.918  
**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	0.900	1.000
CB 3.19.2	31.760	33.632	13.629	0.891	1.000
CG 3.19.3	27.613	28.412	13.801	1.000	1.000
CD 3.19.4	50.991	49.797	3.175	0.918	1.000
N	NA	—	—	0.000	0.000
HA 3.19.5	4.396	4.332	0.427	0.800	1.000
HB2 3.19.6	1.831	2.099	0.501	0.891	1.000
HB3 3.19.7	2.453	2.052	0.596	1.000	1.000
HG2 3.19.8	2.032	1.927	0.364	0.881	1.000
HG3 3.19.9	1.885	1.907	0.417	1.000	1.000
HD2 3.19.10	3.845	3.640	0.682	0.910	1.000
HD3 3.19.11	3.616	3.558	0.522	0.910	1.000

#### 3.19.1 Detailed Probabilities of PRO19CA:

**Overall probability:** 0.900  
**Overall confidence:** 1.000

#### Inter- and intra-residue probability

Residue	Probability	Confidence
THR18	1.00	1.00
PRO19	1.00	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	0.019	1.00	0.00
PRO19	HA	1.00	0.000	1.00	0.00
PRO19	HB2	1.00	0.000	1.00	0.00
PRO19	HB3	1.00	0.000	1.00	0.00
PRO19	HG2	1.00	0.000	1.00	0.00
PRO19	HG3	1.00	0.000	1.00	0.00
PRO19	HD2	1.00	0.000	1.00	0.00
PRO19	HD3	1.00	0.000	1.00	0.00
ASN20	HA	1.00	0.228	0.00	0.00
ASN20	H	1.00	0.000	1.00	0.00

**3.19.2 Detailed Probabilities of PRO19CB:**

Overall probability: 0.891

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO19	1.00	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**

## 3.19 PRO(19)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PRO19	HA	1.00	0.000	1.00	0.00
PRO19	HB2	1.00	0.000	1.00	0.00
PRO19	HB3	1.00	0.000	1.00	0.00
PRO19	HG2	1.00	0.000	1.00	0.00
PRO19	HG3	1.00	0.000	1.00	0.00
PRO19	HD2	1.00	0.000	1.00	0.00
PRO19	HD3	1.00	0.000	1.00	0.00
ASN20	HA	0.98	0.789	0.02	0.00
ASN20	H	1.00	0.000	1.00	0.00

## 3.19.3 Detailed Probabilities of PRO19CG:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
THR18	1.00	1.00
PRO19	1.00	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	0.001	1.00	0.00
PRO19	HA	1.00	0.000	1.00	0.00
PRO19	HB2	1.00	0.000	1.00	0.00
PRO19	HB3	1.00	0.000	1.00	0.00
PRO19	HG2	1.00	0.000	1.00	0.00
PRO19	HG3	1.00	0.000	1.00	0.00
PRO19	HD2	1.00	0.000	1.00	0.00
PRO19	HD3	1.00	0.000	1.00	0.00

## 3.19.4 Detailed Probabilities of PRO19CD:

Overall probability: 0.918

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
THR18	0.78	1.00
PRO19	1.00	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	0.005	1.00	0.00
THR18	HB	0.99	0.003	1.00	0.00
THR18	H	1.00	0.039	0.10	0.00
THR18	HG21	0.94	0.001	1.00	0.00
PRO19	HA	1.00	0.000	1.00	0.00
PRO19	HB2	1.00	0.000	1.00	0.00
PRO19	HB3	1.00	0.000	1.00	0.00
PRO19	HG2	1.00	0.000	1.00	0.00
PRO19	HG3	1.00	0.000	1.00	0.00
PRO19	HD2	1.00	0.000	1.00	0.00
PRO19	HD3	1.00	0.000	1.00	0.00

**3.19.5 Detailed Probabilities of PRO19HA:**

Overall probability: 0.800

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR18	0.00	1.00
PRO19	1.00	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	0.112	0.00	0.00
PRO19	HA	1.00	0.000	1.00	0.00
PRO19	HB2	1.00	0.000	1.00	0.00
PRO19	HB3	1.00	0.000	1.00	0.00
PRO19	HG2	1.00	0.000	1.00	0.00
PRO19	HG3	1.00	0.000	1.00	0.00
PRO19	HD2	1.00	0.000	1.00	0.00
PRO19	HD3	1.00	0.000	1.00	0.00
ASN20	HA	1.00	0.413	0.00	0.00
ASN20	H	1.00	0.000	1.00	0.00

**3.19.6 Detailed Probabilities of PRO19HB2:**

Overall probability: 0.891

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO19	1.00	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	0.000	1.00	0.00
PRO19	HB2	1.00	0.000	1.00	0.00
PRO19	HB3	1.00	0.000	1.00	0.00
PRO19	HG2	1.00	0.000	1.00	0.00
PRO19	HG3	1.00	0.000	1.00	0.00
PRO19	HD2	1.00	0.000	1.00	0.00
PRO19	HD3	1.00	0.000	1.00	0.00
ASN20	HA	0.98	0.173	0.02	0.00
ASN20	H	1.00	0.000	1.00	0.00

**3.19.7 Detailed Probabilities of PRO19HB3:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO19	1.00	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	0.000	1.00	0.00
PRO19	HB2	1.00	0.000	1.00	0.00
PRO19	HB3	1.00	0.000	1.00	0.00
PRO19	HG2	1.00	0.000	1.00	0.00
PRO19	HG3	1.00	0.000	1.00	0.00
PRO19	HD2	1.00	0.000	1.00	0.00
PRO19	HD3	1.00	0.000	1.00	0.00
ASN20	H	1.00	0.000	1.00	0.00

**3.19.8 Detailed Probabilities of PRO19HG2:**

Overall probability: 0.881

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR18	0.05	1.00
PRO19	1.00	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	0.063	0.05	0.00
PRO19	HA	1.00	0.000	1.00	0.00
PRO19	HB2	1.00	0.000	1.00	0.00
PRO19	HB3	1.00	0.000	1.00	0.00
PRO19	HG2	1.00	0.000	1.00	0.00
PRO19	HG3	1.00	0.000	1.00	0.00
PRO19	HD2	1.00	0.000	1.00	0.00
PRO19	HD3	1.00	0.000	1.00	0.00

**3.19.9 Detailed Probabilities of PRO19HG3:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO19	1.00	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	0.000	1.00	0.00
PRO19	HB2	1.00	0.000	1.00	0.00
PRO19	HB3	1.00	0.000	1.00	0.00
PRO19	HG2	1.00	0.000	1.00	0.00
PRO19	HG3	1.00	0.000	1.00	0.00
PRO19	HD2	1.00	0.000	1.00	0.00
PRO19	HD3	1.00	0.000	1.00	0.00

**3.19.10 Detailed Probabilities of PRO19HD2:**

Overall probability: 0.910

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR18	0.75	1.00
PRO19	1.00	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	0.007	1.00	0.00
THR18	HB	0.99	0.005	1.00	0.00
THR18	H	1.00	0.663	0.00	0.00
THR18	HG21	0.94	0.001	1.00	0.00
PRO19	HA	1.00	0.000	1.00	0.00
PRO19	HB2	1.00	0.000	1.00	0.00
PRO19	HB3	1.00	0.000	1.00	0.00
PRO19	HG2	1.00	0.000	1.00	0.00
PRO19	HG3	1.00	0.000	1.00	0.00
PRO19	HD2	1.00	0.000	1.00	0.00
PRO19	HD3	1.00	0.000	1.00	0.00

**3.19.11 Detailed Probabilities of PRO19HD3:**

Overall probability: 0.910

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR18	0.75	1.00
PRO19	1.00	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	0.006	1.00	0.00
THR18	HB	0.99	0.010	1.00	0.00
THR18	H	0.99	0.892	0.01	0.00
THR18	HG21	0.79	0.010	1.00	0.00
PRO19	HA	1.00	0.000	1.00	0.00
PRO19	HB2	1.00	0.000	1.00	0.00
PRO19	HB3	1.00	0.000	1.00	0.00
PRO19	HG2	1.00	0.000	1.00	0.00
PRO19	HG3	1.00	0.000	1.00	0.00
PRO19	HD2	1.00	0.000	1.00	0.00
PRO19	HD3	1.00	0.000	1.00	0.00

### L-Asparagine (Asn)

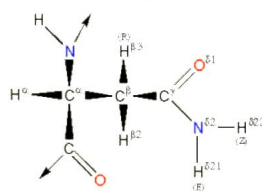


Figure 10: Image from the BMRB

Residue probability confidence: 1.000

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	0.575	1.000
CB 3.20.2	40.042	38.785	5.449	1.000	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	0.694	1.000
HB2 3.20.6	2.911	2.800	0.341	1.000	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	0.703	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	0.880	1.000

## Overall confidence: 1.000

Residue	Probability	Confidence
PRO19	0.34	1.00
ASN20	0.73	1.00
PRO21	0.51	1.00

## Residues TOC

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	0.413	0.00	0.00
PRO19	HB2	0.98	0.173	0.02	0.00
PRO19	HG2	0.65	0.028	1.00	0.00
ASN20	HA	1.00	0.000	1.00	0.00
ASN20	HB2	1.00	0.000	1.00	0.00
ASN20	HB3	1.00	0.000	1.00	0.00
ASN20	H	1.00	0.000	1.00	0.00
ASN20	HD21	1.00	0.394	0.00	0.00
ASN20	HD22	1.00	0.036	0.40	0.00
PRO21	HA	1.00	0.573	0.00	0.00
PRO21	HG2	0.95	0.100	0.05	0.00
PRO21	HD2	1.00	0.004	1.00	0.00
PRO21	HG3	0.93	0.015	1.00	0.00

**3.20.2 Detailed Probabilities of ASN20CB:**

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
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	0.000	1.00	0.00
ASN20	HB2	1.00	0.000	1.00	0.00
ASN20	HB3	1.00	0.000	1.00	0.00
ASN20	H	1.00	0.000	1.00	0.00
ASN20	HD21	1.00	0.000	1.00	0.00
ASN20	HD22	1.00	0.000	1.00	0.00
PRO21	HD2	0.98	0.007	1.00	0.00

**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	0.000	1.00	0.00
PRO19	HB2	1.00	0.000	1.00	0.00
PRO19	HB3	1.00	0.000	1.00	0.00
PRO19	HG2	0.95	0.000	1.00	0.00
PRO19	HG3	0.84	0.000	1.00	0.00
PRO19	HD2	0.77	0.000	1.00	0.00
PRO19	HD3	0.71	0.000	1.00	0.00
ASN20	HA	1.00	0.000	1.00	0.00
ASN20	HB2	1.00	0.000	1.00	0.00
ASN20	HB3	1.00	0.000	1.00	0.00
ASN20	H	1.00	0.000	1.00	0.00
ASN20	HD21	0.98	0.586	0.02	0.00
PRO21	HD2	1.00	0.004	1.00	0.00

**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	0.001	1.00	0.00
ASN20	HB2	1.00	0.000	1.00	0.00
ASN20	HB3	1.00	0.000	1.00	0.00
ASN20	HD21	1.00	0.000	1.00	0.00
ASN20	HD22	1.00	0.000	1.00	0.00

**3.20.5 Detailed Probabilities of ASN20HA:**

Overall probability: 0.694

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO19	0.01	1.00
ASN20	0.83	1.00
PRO21	0.80	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	0.228	0.00	0.00
PRO19	HB2	0.98	0.789	0.02	0.00
ASN20	HA	1.00	0.000	1.00	0.00
ASN20	HB2	1.00	0.000	1.00	0.00
ASN20	HB3	1.00	0.000	1.00	0.00
ASN20	H	1.00	0.000	1.00	0.00
ASN20	HD21	1.00	2.060	0.00	0.00
ASN20	HD22	1.00	0.001	1.00	0.00
PRO21	HA	1.00	0.213	0.00	0.00
PRO21	HG2	0.95	0.001	1.00	0.00
PRO21	HD2	1.00	0.003	1.00	0.00
PRO21	HB3	0.80	0.001	1.00	0.00
PRO21	HG3	0.93	0.003	1.00	0.00

**3.20.6 Detailed Probabilities of ASN20HB2:**

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
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	0.000	1.00	0.00
ASN20	HB2	1.00	0.000	1.00	0.00
ASN20	HB3	1.00	0.000	1.00	0.00
ASN20	H	1.00	0.000	1.00	0.00
ASN20	HD21	1.00	0.000	1.00	0.00
ASN20	HD22	1.00	0.000	1.00	0.00
PRO21	HD2	0.98	0.004	1.00	0.00

**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	0.000	1.00	0.00
ASN20	HB2	1.00	0.000	1.00	0.00
ASN20	HB3	1.00	0.000	1.00	0.00
ASN20	H	1.00	0.000	1.00	0.00
ASN20	HD21	1.00	0.000	1.00	0.00
ASN20	HD22	1.00	0.000	1.00	0.00
PRO21	HD2	0.98	0.010	1.00	0.00

**3.20.8 Detailed Probabilities of ASN20H:**

Overall probability: 0.703

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO19	0.75	1.00
ASN20	0.80	1.00
PRO21	0.00	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	0.000	1.00	0.00
PRO19	HB2	1.00	0.000	1.00	0.00
PRO19	HB3	1.00	3.435	0.00	0.00
PRO19	HD3	0.71	0.000	1.00	0.00
ASN20	HA	1.00	0.000	1.00	0.00
ASN20	HB2	1.00	0.000	1.00	0.00
ASN20	HB3	1.00	0.000	1.00	0.00
ASN20	H	1.00	0.000	1.00	0.00
ASN20	HD21	0.98	0.228	0.02	0.00
PRO21	HD2	1.00	0.608	0.00	0.00

**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	0.394	0.00	0.00
ASN20	HB2	1.00	0.000	1.00	0.00
ASN20	HB3	1.00	0.000	1.00	0.00
ASN20	H	0.98	0.586	0.02	0.00
ASN20	HD21	1.00	0.000	1.00	0.00
ASN20	HD22	1.00	0.000	1.00	0.00

**3.20.10 Detailed Probabilities of ASN20HD22:**

Overall probability: 0.880

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASN20	0.88	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	0.036	0.40	0.00
ASN20	HB2	1.00	0.000	1.00	0.00
ASN20	HB3	1.00	0.000	1.00	0.00
ASN20	HD21	1.00	0.000	1.00	0.00
ASN20	HD22	1.00	0.000	1.00	0.00

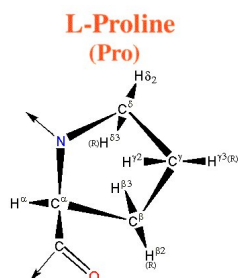
**3.21 PRO(21)**

Figure 11: Image from the BMRB

Residue probability: 0.899

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	0.667	1.000
CB 3.21.2	32.124	33.632	13.629	1.000	1.000
CG 3.21.3	27.140	28.412	13.801	1.000	1.000
CD 3.21.4	51.083	49.797	3.175	0.901	1.000
N	NA	—	—	0.000	0.000
HA 3.21.5	4.612	4.332	0.427	0.778	1.000
HB2 3.21.6	2.018	2.099	0.501	0.878	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	0.864	1.000
HG3 3.21.9	2.019	1.907	0.417	1.000	1.000
HD 3.21.10	3.987	3.640	0.682	0.900	1.000

**3.21.1 Detailed Probabilities of PRO21CA:**

Overall probability: 0.667

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASN20	0.00	1.00
PRO21	0.83	1.00
ASN22	0.50	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	0.213	0.00	0.00
PRO21	HA	1.00	0.000	1.00	0.00
PRO21	HB2	1.00	0.000	1.00	0.00
PRO21	HB3	1.00	0.000	1.00	0.00
PRO21	HG2	1.00	0.000	1.00	0.00
PRO21	HG3	1.00	0.000	1.00	0.00
PRO21	HD2	1.00	0.052	0.00	0.00
ASN22	HA	1.00	0.091	0.00	0.00
ASN22	H	1.00	0.000	1.00	0.00

**3.21.2 Detailed Probabilities of PRO21CB:**

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
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	0.00
PRO21	HB2	1.00	0.000	1.00	0.00
PRO21	HB3	1.00	0.000	1.00	0.00
PRO21	HG2	1.00	0.000	1.00	0.00
PRO21	HG3	1.00	0.000	1.00	0.00
PRO21	HD2	1.00	0.000	1.00	0.00
ASN22	HA	0.98	0.000	1.00	0.00
ASN22	H	1.00	0.000	1.00	0.00
ASN22	HB2	0.56	0.015	1.00	0.00

**3.21.3 Detailed Probabilities of PRO21CG:**

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	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	0.00
PRO21	HA	1.00	0.000	1.00	0.00
PRO21	HB2	1.00	0.000	1.00	0.00
PRO21	HB3	1.00	0.000	1.00	0.00
PRO21	HG2	1.00	0.000	1.00	0.00
PRO21	HG3	1.00	0.000	1.00	0.00
PRO21	HD2	1.00	0.000	1.00	0.00

**3.21.4 Detailed Probabilities of PRO21CD:**

Overall probability: 0.901

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASN20	0.75	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	0.003	1.00	0.00
ASN20	HB2	0.98	0.004	1.00	0.00
ASN20	HB3	0.99	0.010	1.00	0.00
ASN20	H	0.99	0.608	0.01	0.00
PRO21	HA	1.00	0.000	1.00	0.00
PRO21	HB2	1.00	0.000	1.00	0.00
PRO21	HB3	1.00	0.000	1.00	0.00
PRO21	HG2	1.00	0.000	1.00	0.00
PRO21	HG3	1.00	0.000	1.00	0.00
PRO21	HD2	1.00	0.000	1.00	0.00

**3.21.5 Detailed Probabilities of PRO21HA:**

Overall probability: 0.778

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASN20	0.00	1.00
PRO21	1.00	1.00
ASN22	0.50	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	0.573	0.00	0.00
PRO21	HA	1.00	0.000	1.00	0.00
PRO21	HB2	1.00	0.000	1.00	0.00
PRO21	HB3	1.00	0.000	1.00	0.00
PRO21	HG2	1.00	0.000	1.00	0.00
PRO21	HG3	1.00	0.000	1.00	0.00
PRO21	HD2	1.00	0.000	1.00	0.00
ASN22	HA	1.00	0.269	0.00	0.00
ASN22	H	1.00	0.000	1.00	0.00

**3.21.6 Detailed Probabilities of PRO21HB2:**

Overall probability: 0.878

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO21	1.00	1.00
ASN22	0.51	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	0.00
PRO21	HB2	1.00	0.000	1.00	0.00
PRO21	HB3	1.00	0.000	1.00	0.00
PRO21	HG2	1.00	0.000	1.00	0.00
PRO21	HG3	1.00	0.000	1.00	0.00
PRO21	HD2	1.00	0.000	1.00	0.00
ASN22	HA	0.98	0.718	0.02	0.00
ASN22	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
PRO21	HB2	1.00	0.000	1.00	0.00
PRO21	HB3	1.00	0.000	1.00	0.00
PRO21	HG2	1.00	0.000	1.00	0.00
PRO21	HG3	1.00	0.000	1.00	0.00
PRO21	HD2	1.00	0.000	1.00	0.00
ASN22	H	1.00	0.000	1.00	0.00

**3.21.8 Detailed Probabilities of PRO21HG2:**

Overall probability: 0.864

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASN20	0.05	1.00
PRO21	1.00	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	0.100	0.05	0.00
PRO21	HA	1.00	0.000	1.00	0.00
PRO21	HB2	1.00	0.000	1.00	0.00
PRO21	HB3	1.00	0.000	1.00	0.00
PRO21	HG2	1.00	0.000	1.00	0.00
PRO21	HG3	1.00	0.000	1.00	0.00
PRO21	HD2	1.00	0.000	1.00	0.00

**3.21.9 Detailed Probabilities of PRO21HG3:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO21	1.00	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	0.000	1.00	0.00
PRO21	HB2	1.00	0.000	1.00	0.00
PRO21	HB3	1.00	0.000	1.00	0.00
PRO21	HG2	1.00	0.000	1.00	0.00
PRO21	HG3	1.00	0.000	1.00	0.00
PRO21	HD2	1.00	0.000	1.00	0.00

**3.21.10 Detailed Probabilities of PRO21HD2:**

Overall probability: 0.900

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASN20	1.00	1.00
PRO21	0.83	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	0.004	1.00	0.00
ASN20	HB2	0.98	0.007	1.00	0.00
ASN20	HB3	0.99	0.007	1.00	0.00
ASN20	H	0.99	0.004	1.00	0.00
PRO21	HA	1.00	0.052	0.00	0.00
PRO21	HB2	1.00	0.000	1.00	0.00
PRO21	HB3	1.00	0.000	1.00	0.00
PRO21	HG2	1.00	0.000	1.00	0.00
PRO21	HG3	1.00	0.000	1.00	0.00
PRO21	HD2	1.00	0.000	1.00	0.00

**3.22 ASN(22)**

Figure 12: Image from the BMRB

Residue probability: 0.859

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	0.502	1.000
CB 3.22.2	38.310	38.785	5.449	1.000	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	0.837	1.000
HA 3.22.5	4.881	4.658	0.371	0.700	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	1.000	1.000
H 3.22.8	8.439	8.328	0.633	0.919	1.000
HD21 3.22.9	7.270	7.343	1.188	0.833	1.000
HD22 3.22.10	6.280	7.145	1.184	0.800	1.000

**3.22.1 Detailed Probabilities of ASN22CA:**

Overall probability: 0.502

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO21	0.01	1.00
ASN22	0.67	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	0.269	0.00	0.00
PRO21	HB2	0.98	0.718	0.02	0.00
ASN22	HA	1.00	0.000	1.00	0.00
ASN22	HB2	1.00	0.000	1.00	0.00
ASN22	HB3	1.00	0.000	1.00	0.00
ASN22	H	1.00	0.000	1.00	0.00
ASN22	HD21	1.00	1.169	0.00	0.00
ASN22	HD22	1.00	1.399	0.00	0.00
SER23	HA	1.00	1.286	0.00	0.00
SER23	H	1.00	0.000	1.00	0.00

**3.22.2 Detailed Probabilities of ASN22CB:**

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	0.000	1.00	0.00
ASN22	HB2	1.00	0.000	1.00	0.00
ASN22	HB3	1.00	0.000	1.00	0.00
ASN22	H	1.00	0.000	1.00	0.00
ASN22	HD21	1.00	0.000	1.00	0.00
ASN22	HD22	1.00	0.000	1.00	0.00
SER23	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
PRO21	HB2	1.00	0.000	1.00	0.00
PRO21	HB3	1.00	0.000	1.00	0.00
PRO21	HG2	0.95	0.000	1.00	0.00
PRO21	HG3	0.84	0.000	1.00	0.00
PRO21	HD2	0.77	0.000	1.00	0.00
ASN22	HA	1.00	0.000	1.00	0.00
ASN22	HB2	1.00	0.000	1.00	0.00
ASN22	HB3	1.00	0.000	1.00	0.00
ASN22	H	1.00	0.000	1.00	0.00
ASN22	HD21	0.98	0.000	1.00	0.00
SER23	H	1.00	0.000	1.00	0.00

**3.22.4 Detailed Probabilities of ASN22ND2:**

Overall probability: 0.837

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASN22	0.84	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	0.000	1.00	0.00
ASN22	HB2	1.00	0.000	1.00	0.00
ASN22	HB3	1.00	0.000	1.00	0.00
ASN22	H	0.98	1.169	0.02	0.00
ASN22	HD21	1.00	0.000	1.00	0.00
ASN22	HD22	1.00	0.000	1.00	0.00

**3.22.5 Detailed Probabilities of ASN22HA:**

Overall probability: 0.700

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO21	0.50	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	0.091	0.00	0.00
PRO21	HB2	0.98	0.000	1.00	0.00
ASN22	HA	1.00	0.000	1.00	0.00
ASN22	HB2	1.00	0.000	1.00	0.00
ASN22	HB3	1.00	0.000	1.00	0.00
ASN22	H	1.00	0.000	1.00	0.00
ASN22	HD21	1.00	0.000	1.00	0.00
ASN22	HD22	1.00	0.187	0.00	0.00
SER23	HA	1.00	0.955	0.00	0.00
SER23	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ASN22	HB2	1.00	0.000	1.00	0.00
ASN22	HB3	1.00	0.000	1.00	0.00
ASN22	H	1.00	0.000	1.00	0.00
ASN22	HD21	1.00	0.000	1.00	0.00
ASN22	HD22	1.00	0.000	1.00	0.00
SER23	H	1.00	0.000	1.00	0.00

**3.22.7 Detailed Probabilities of ASN22HB3:**

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
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	0.000	1.00	0.00
ASN22	HB2	1.00	0.000	1.00	0.00
ASN22	HB3	1.00	0.000	1.00	0.00
ASN22	H	1.00	0.000	1.00	0.00
ASN22	HD21	1.00	0.000	1.00	0.00
ASN22	HD22	1.00	0.000	1.00	0.00
SER23	H	1.00	0.000	1.00	0.00

**3.22.8 Detailed Probabilities of ASN22H:**

Overall probability: 0.919

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO21	1.00	1.00
ASN22	0.80	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	0.000	1.00	0.00
PRO21	HB2	1.00	0.000	1.00	0.00
PRO21	HB3	1.00	0.000	1.00	0.00
PRO21	HG2	0.95	0.000	1.00	0.00
PRO21	HG3	0.84	0.000	1.00	0.00
PRO21	HD2	0.77	0.000	1.00	0.00
ASN22	HA	1.00	0.000	1.00	0.00
ASN22	HB2	1.00	0.000	1.00	0.00
ASN22	HB3	1.00	0.000	1.00	0.00
ASN22	H	1.00	0.000	1.00	0.00
ASN22	HD21	0.98	1.169	0.02	0.00
SER23	H	1.00	0.000	1.00	0.00

**3.22.9 Detailed Probabilities of ASN22HD21:**

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
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	1.169	0.00	0.00
ASN22	HB2	1.00	0.000	1.00	0.00
ASN22	HB3	1.00	0.000	1.00	0.00
ASN22	H	0.98	0.000	1.00	0.00
ASN22	HD21	1.00	0.000	1.00	0.00
ASN22	HD22	1.00	0.000	1.00	0.00

**3.22.10 Detailed Probabilities of ASN22HD22:**

Overall probability: 0.800

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASN22	0.80	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	1.399	0.00	0.00
ASN22	HB2	1.00	0.000	1.00	0.00
ASN22	HB3	1.00	0.000	1.00	0.00
ASN22	HD21	1.00	0.000	1.00	0.00
ASN22	HD22	1.00	0.000	1.00	0.00

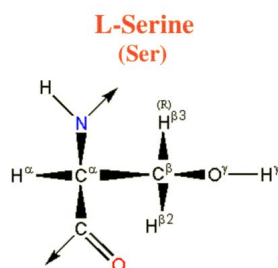
**3.23 SER(23)**

Figure 13: Image from the BMRB

Residue probability: 0.918

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	0.714	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	1.000	0.900
HA 3.23.4	6.167	4.486	0.430	0.714	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	1.000	0.833
H 3.23.7	8.555	8.292	0.600	1.000	0.900
HG	NA	—	—	0.000	0.000

**3.23.1 Detailed Probabilities of SER23CA:**

Overall probability: 0.714

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASN22	0.00	1.00
SER23	1.00	0.80
LEU24	0.50	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	0.955	0.00	0.00
SER23	HA	1.00	0.000	1.00	0.00
SER23	HB2	1.00	0.000	1.00	0.00
SER23	HB3	1.00	0.000	1.00	0.00
SER23	H	1.00	0.000	1.00	0.00
LEU24	HA	1.00	0.725	0.00	0.00
LEU24	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
SER23	HB2	1.00	0.000	1.00	0.00
SER23	HB3	1.00	0.000	1.00	0.00
SER23	H	1.00	0.000	1.00	0.00
LEU24	H	1.00	0.000	1.00	0.00

**3.23.3 Detailed Probabilities of SER23N:**

Overall probability: 1.000

Overall confidence: 0.900

**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
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	0.00
ASN22	HB2	1.00	0.000	1.00	0.00
ASN22	HB3	1.00	0.000	1.00	0.00
ASN22	H	1.00	0.000	1.00	0.00
SER23	HA	1.00	0.000	1.00	0.00
SER23	HB2	1.00	0.000	1.00	0.00
SER23	HB3	1.00	0.000	1.00	0.00
SER23	H	1.00	0.000	1.00	0.00
LEU24	H	1.00	0.000	1.00	0.00

**3.23.4 Detailed Probabilities of SER23HA:**

Overall probability: 0.714

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASN22	0.00	1.00
SER23	1.00	0.80
LEU24	0.50	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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN22	HA	1.00	1.286	0.00	0.00
SER23	HA	1.00	0.000	1.00	0.00
SER23	HB2	1.00	0.000	1.00	0.00
SER23	HB3	1.00	0.000	1.00	0.00
SER23	H	1.00	0.000	1.00	0.00
LEU24	HA	1.00	1.705	0.00	0.00
LEU24	H	1.00	0.000	1.00	0.00

#### 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	0.000	1.00	0.00
SER23	HB2	1.00	0.000	1.00	0.00
SER23	HB3	1.00	0.000	1.00	0.00
SER23	H	1.00	0.000	1.00	0.00
LEU24	H	1.00	0.000	1.00	0.00

#### 3.23.6 Detailed Probabilities of SER23HB3:

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
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	0.000	1.00	0.00
SER23	HB2	1.00	0.000	1.00	0.00
SER23	HB3	1.00	0.000	1.00	0.00
SER23	H	1.00	0.000	1.00	0.00
LEU24	H	1.00	0.000	1.00	0.00

**3.23.7 Detailed Probabilities of SER23H:**

Overall probability: 1.000

Overall confidence: 0.900

**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
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	0.00
ASN22	HB2	1.00	0.000	1.00	0.00
ASN22	HB3	1.00	0.000	1.00	0.00
ASN22	H	1.00	0.000	1.00	0.00
SER23	HA	1.00	0.000	1.00	0.00
SER23	HB2	1.00	0.000	1.00	0.00
SER23	HB3	1.00	0.000	1.00	0.00
SER23	H	1.00	0.000	1.00	0.00
LEU24	H	1.00	0.000	1.00	0.00

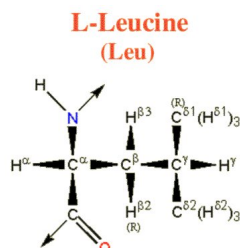
**3.24 LEU(24)**

Figure 14: Image from the BMRB

Residue probability: 0.969

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	0.800	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	1.000	1.000
CD1 3.24.4	23.238	24.837	3.657	1.000	1.000
CD2 3.24.5	24.100	24.201	3.117	1.000	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	0.800	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	1.000	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	1.000	1.000
HD2 3.24.12	0.029	0.727	0.421	1.000	1.000
H 3.24.13	8.732	8.237	0.647	1.000	0.909

**3.24.1 Detailed Probabilities of LEU24CA:**

Overall probability: 0.800

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER23	0.00	1.00
LEU24	1.00	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	1.705	0.00	0.00
LEU24	HA	1.00	0.000	1.00	0.00
LEU24	HB2	1.00	0.000	1.00	0.00
LEU24	HB3	1.00	0.000	1.00	0.00
LEU24	HG	1.00	0.000	1.00	0.00
LEU24	HD11	0.99	0.000	1.00	0.00
LEU24	HD21	0.99	0.000	1.00	0.00
LEU24	H	1.00	0.000	1.00	0.00
LYS25	HA	1.00	0.385	0.00	0.00
LYS25	H	1.00	0.000	1.00	0.00

**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	0.00
LEU24	HB2	1.00	0.000	1.00	0.00
LEU24	HB3	1.00	0.000	1.00	0.00
LEU24	HG	1.00	0.000	1.00	0.00
LEU24	HD11	1.00	0.000	1.00	0.00
LEU24	HD21	1.00	0.000	1.00	0.00
LEU24	H	1.00	0.000	1.00	0.00
LYS25	H	1.00	0.000	1.00	0.00

## 3.24.3 Detailed Probabilities of LEU24CG:

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	0.000	1.00	0.00
LEU24	HB2	1.00	0.000	1.00	0.00
LEU24	HB3	1.00	0.000	1.00	0.00
LEU24	HG	1.00	0.000	1.00	0.00
LEU24	HD11	1.00	0.000	1.00	0.00
LEU24	HD21	1.00	0.000	1.00	0.00
LEU24	H	1.00	0.000	1.00	0.00
LYS25	H	0.98	0.000	1.00	0.00

## 3.24.4 Detailed Probabilities of LEU24CD1:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
LEU24	1.00	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	0.000	1.00	0.00
LEU24	HB2	1.00	0.000	1.00	0.00
LEU24	HB3	1.00	0.000	1.00	0.00
LEU24	HG	1.00	0.000	1.00	0.00
LEU24	HD11	1.00	0.000	1.00	0.00
LEU24	HD21	1.00	0.000	1.00	0.00
LEU24	H	0.86	0.000	1.00	0.00

**3.24.5 Detailed Probabilities of LEU24CD2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU24	1.00	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	0.000	1.00	0.00
LEU24	HB2	1.00	0.000	1.00	0.00
LEU24	HB3	1.00	0.000	1.00	0.00
LEU24	HG	1.00	0.000	1.00	0.00
LEU24	HD11	1.00	0.000	1.00	0.00
LEU24	HD21	1.00	0.000	1.00	0.00
LEU24	H	0.85	0.000	1.00	0.00

**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	0.000	1.00	0.00
SER23	HB2	1.00	0.000	1.00	0.00
SER23	HB3	1.00	0.000	1.00	0.00
SER23	H	1.00	0.000	1.00	0.00
LEU24	HA	1.00	0.000	1.00	0.00
LEU24	HB2	1.00	0.000	1.00	0.00
LEU24	HB3	1.00	0.000	1.00	0.00
LEU24	HG	1.00	0.000	1.00	0.00
LEU24	H	1.00	0.000	1.00	0.00
LEU24	HD11	0.88	0.000	1.00	0.00
LEU24	HD21	0.87	0.000	1.00	0.00
LYS25	H	1.00	0.000	1.00	0.00

**3.24.7 Detailed Probabilities of LEU24HA:**

Overall probability: 0.800

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER23	0.00	1.00
LEU24	1.00	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	0.725	0.00	0.00
LEU24	HA	1.00	0.000	1.00	0.00
LEU24	HB2	1.00	0.000	1.00	0.00
LEU24	HB3	1.00	0.000	1.00	0.00
LEU24	HG	1.00	0.000	1.00	0.00
LEU24	HD11	0.99	0.000	1.00	0.00
LEU24	HD21	0.99	0.000	1.00	0.00
LEU24	H	1.00	0.000	1.00	0.00
LYS25	HA	1.00	0.385	0.00	0.00
LYS25	H	1.00	0.000	1.00	0.00

**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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU24	HA	1.00	0.000	1.00	0.00
LEU24	HB2	1.00	0.000	1.00	0.00
LEU24	HB3	1.00	0.000	1.00	0.00
LEU24	HG	1.00	0.000	1.00	0.00
LEU24	HD11	1.00	0.000	1.00	0.00
LEU24	HD21	1.00	0.000	1.00	0.00
LEU24	H	1.00	0.000	1.00	0.00
LYS25	H	1.00	0.000	1.00	0.00

## 3.24.9 Detailed Probabilities of LEU24HB3:

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
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	0.000	1.00	0.00
LEU24	HB2	1.00	0.000	1.00	0.00
LEU24	HB3	1.00	0.000	1.00	0.00
LEU24	HG	1.00	0.000	1.00	0.00
LEU24	HD11	1.00	0.000	1.00	0.00
LEU24	HD21	1.00	0.000	1.00	0.00
LEU24	H	1.00	0.000	1.00	0.00
LYS25	H	1.00	0.000	1.00	0.00

## 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	0.000	1.00	0.00
LEU24	HB2	1.00	0.000	1.00	0.00
LEU24	HB3	1.00	0.000	1.00	0.00
LEU24	HG	1.00	0.000	1.00	0.00
LEU24	HD11	1.00	0.000	1.00	0.00
LEU24	HD21	1.00	0.000	1.00	0.00
LEU24	H	1.00	0.000	1.00	0.00
LYS25	H	0.98	0.000	1.00	0.00

**3.24.11 Detailed Probabilities of LEU24HD11:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU24	1.00	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	0.000	1.00	0.00
LEU24	HB2	1.00	0.000	1.00	0.00
LEU24	HB3	1.00	0.000	1.00	0.00
LEU24	HG	1.00	0.000	1.00	0.00
LEU24	HD11	1.00	0.000	1.00	0.00
LEU24	HD21	1.00	0.000	1.00	0.00
LEU24	H	0.86	0.000	1.00	0.00

**3.24.12 Detailed Probabilities of LEU24HD21:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU24	1.00	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	0.000	1.00	0.00
LEU24	HB2	1.00	0.000	1.00	0.00
LEU24	HB3	1.00	0.000	1.00	0.00
LEU24	HG	1.00	0.000	1.00	0.00
LEU24	HD11	1.00	0.000	1.00	0.00
LEU24	HD21	1.00	0.000	1.00	0.00
LEU24	H	0.85	0.000	1.00	0.00

**3.24.13 Detailed Probabilities of LEU24H:**

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	0.000	1.00	0.00
SER23	HB2	1.00	0.000	1.00	0.00
SER23	HB3	1.00	0.000	1.00	0.00
SER23	H	1.00	0.000	1.00	0.00
LEU24	HA	1.00	0.000	1.00	0.00
LEU24	HB2	1.00	0.000	1.00	0.00
LEU24	HB3	1.00	0.000	1.00	0.00
LEU24	HG	1.00	0.000	1.00	0.00
LEU24	H	1.00	0.000	1.00	0.00
LEU24	HD11	0.88	0.000	1.00	0.00
LEU24	HD21	0.87	0.000	1.00	0.00
LYS25	H	1.00	0.000	1.00	0.00

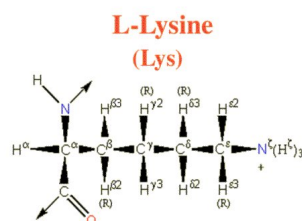


Figure 15: Image from the BMRB

Residue probability: 0.965  
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	0.800	1.000
CB 3.25.2	34.585	32.981	3.186	1.000	1.000
CG 3.25.3	25.106	24.941	1.956	1.000	0.909
CD 3.25.4	29.299	29.020	2.193	1.000	0.889
CE 3.25.5	41.649	41.893	1.492	1.000	0.875
N 3.25.6	123.734	120.954	4.210	0.875	1.000
NZ	NA	—	—	0.000	0.000
HA 3.25.7	4.847	4.262	0.489	0.900	1.000
HB2 3.25.8	1.523	1.774	0.365	1.000	1.000
HB3 3.25.9	1.637	1.742	0.385	1.000	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	0.900	0.909
HD 3.25.12	1.563	1.614	0.957	1.000	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	1.000	1.000
HZ	NA	—	—	0.000	0.000

**3.25.1 Detailed Probabilities of LYS25CA:**

Overall probability: 0.800  
Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU24	0.00	1.00
LYS25	1.00	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	0.385	0.00	0.00
LYS25	HA	1.00	0.000	1.00	0.00
LYS25	HB2	1.00	0.000	1.00	0.00
LYS25	HB3	1.00	0.000	1.00	0.00
LYS25	HG2	1.00	0.000	1.00	0.00
LYS25	HG3	1.00	0.000	1.00	0.00
LYS25	HD2	0.98	0.000	1.00	0.00
LYS25	H	1.00	0.000	1.00	0.00
PHE26	HA	1.00	0.012	1.00	0.00
PHE26	H	1.00	1.571	0.00	0.00

**3.25.2 Detailed Probabilities of LYS25CB:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS25	1.00	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**

## 3.25 LYS(25)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS25	HA	1.00	0.000	1.00	0.00
LYS25	HB2	1.00	0.000	1.00	0.00
LYS25	HB3	1.00	0.000	1.00	0.00
LYS25	HG2	1.00	0.000	1.00	0.00
LYS25	HG3	1.00	0.000	1.00	0.00
LYS25	HD2	1.00	0.000	1.00	0.00
LYS25	HE2	0.98	0.000	1.00	0.00
LYS25	HE3	0.99	0.000	1.00	0.00
LYS25	H	1.00	0.000	1.00	0.00
PHE26	H	1.00	0.000	1.00	0.00
PHE26	HA	0.65	0.012	1.00	0.00

## 3.25.3 Detailed Probabilities of LYS25CG:

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	0.000	1.00	0.00
LYS25	HB2	1.00	0.000	1.00	0.00
LYS25	HB3	1.00	0.000	1.00	0.00
LYS25	HG2	1.00	0.000	1.00	0.00
LYS25	HG3	1.00	0.000	1.00	0.00
LYS25	HD2	1.00	0.000	1.00	0.00
LYS25	HE2	1.00	0.000	1.00	0.00
LYS25	HE3	1.00	0.000	1.00	0.00
LYS25	H	1.00	0.000	1.00	0.00
PHE26	H	0.98	0.000	1.00	0.00

**3.25.4 Detailed Probabilities of LYS25CD:**

Overall probability: 1.000

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS25	1.00	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	0.000	1.00	0.00
LYS25	HB2	1.00	0.000	1.00	0.00
LYS25	HB3	1.00	0.000	1.00	0.00
LYS25	HG2	1.00	0.000	1.00	0.00
LYS25	HG3	1.00	0.000	1.00	0.00
LYS25	HD2	1.00	0.000	1.00	0.00
LYS25	HE2	1.00	0.000	1.00	0.00
LYS25	HE3	1.00	0.000	1.00	0.00
LYS25	H	0.87	0.000	1.00	0.00

**3.25.5 Detailed Probabilities of LYS25CE:**

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	0.000	1.00	0.00
LYS25	HB3	0.99	0.000	1.00	0.00
LYS25	HG2	1.00	0.000	1.00	0.00
LYS25	HG3	1.00	0.000	1.00	0.00
LYS25	HD2	1.00	0.000	1.00	0.00
LYS25	HE2	1.00	0.000	1.00	0.00
LYS25	HE3	1.00	0.000	1.00	0.00

**3.25.6 Detailed Probabilities of LYS25N:**

Overall probability: 0.875

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU24	1.00	1.00
LYS25	0.86	1.00
PHE26	0.50	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**

## 3.25 LYS(25)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU24	HA	1.00	0.000	1.00	0.00
LEU24	HB2	1.00	0.000	1.00	0.00
LEU24	HB3	1.00	0.000	1.00	0.00
LEU24	HG	0.98	0.000	1.00	0.00
LEU24	H	1.00	0.000	1.00	0.00
LEU24	HD11	0.52	0.000	1.00	0.00
LEU24	HD21	0.59	0.000	1.00	0.00
LYS25	HA	1.00	0.000	1.00	0.00
LYS25	HB2	1.00	0.000	1.00	0.00
LYS25	HB3	1.00	0.000	1.00	0.00
LYS25	HG2	1.00	0.000	1.00	0.00
LYS25	HG3	1.00	0.060	0.00	0.00
LYS25	H	1.00	0.000	1.00	0.00
LYS25	HD2	0.88	0.000	1.00	0.00
PHE26	H	1.00	0.849	0.00	0.00
PHE26	HA	0.92	0.012	1.00	0.00

## 3.25.7 Detailed Probabilities of LYS25HA:

Overall probability: 0.900

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
LEU24	0.00	1.00
LYS25	1.00	1.00
PHE26	1.00	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

## 3.25 LYS(25)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU24	HA	1.00	0.385	0.00	0.00
LYS25	HA	1.00	0.000	1.00	0.00
LYS25	HB2	1.00	0.000	1.00	0.00
LYS25	HB3	1.00	0.000	1.00	0.00
LYS25	HG2	1.00	0.000	1.00	0.00
LYS25	HG3	1.00	0.000	1.00	0.00
LYS25	HD2	0.98	0.000	1.00	0.00
LYS25	H	1.00	0.000	1.00	0.00
PHE26	HA	1.00	0.012	1.00	0.00
PHE26	H	1.00	0.000	1.00	0.00

## 3.25.8 Detailed Probabilities of LYS25HB2:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
LYS25	1.00	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	0.000	1.00	0.00
LYS25	HB2	1.00	0.000	1.00	0.00
LYS25	HB3	1.00	0.000	1.00	0.00
LYS25	HG2	1.00	0.000	1.00	0.00
LYS25	HG3	1.00	0.000	1.00	0.00
LYS25	HD2	1.00	0.000	1.00	0.00
LYS25	HE2	0.98	0.000	1.00	0.00
LYS25	HE3	0.99	0.000	1.00	0.00
LYS25	H	1.00	0.000	1.00	0.00
PHE26	H	1.00	0.000	1.00	0.00

**3.25.9 Detailed Probabilities of LYS25HB3:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS25	1.00	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	0.000	1.00	0.00
LYS25	HB2	1.00	0.000	1.00	0.00
LYS25	HB3	1.00	0.000	1.00	0.00
LYS25	HG2	1.00	0.000	1.00	0.00
LYS25	HG3	1.00	0.000	1.00	0.00
LYS25	HD2	1.00	0.000	1.00	0.00
LYS25	HE2	0.99	0.000	1.00	0.00
LYS25	HE3	0.99	0.000	1.00	0.00
LYS25	H	1.00	0.000	1.00	0.00
PHE26	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
LYS25	HB2	1.00	0.000	1.00	0.00
LYS25	HB3	1.00	0.000	1.00	0.00
LYS25	HG2	1.00	0.000	1.00	0.00
LYS25	HG3	1.00	0.000	1.00	0.00
LYS25	HD2	1.00	0.000	1.00	0.00
LYS25	HE2	1.00	0.000	1.00	0.00
LYS25	HE3	1.00	0.000	1.00	0.00
LYS25	H	1.00	0.000	1.00	0.00
PHE26	H	0.98	0.000	1.00	0.00

**3.25.11 Detailed Probabilities of LYS25HG3:**

Overall probability: 0.900

Overall confidence: 0.909

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS25	0.89	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	0.000	1.00	0.00
LYS25	HB2	1.00	0.000	1.00	0.00
LYS25	HB3	1.00	0.000	1.00	0.00
LYS25	HG2	1.00	0.000	1.00	0.00
LYS25	HG3	1.00	0.000	1.00	0.00
LYS25	HD2	1.00	0.000	1.00	0.00
LYS25	HE2	1.00	0.000	1.00	0.00
LYS25	HE3	1.00	0.000	1.00	0.00
LYS25	H	1.00	0.060	0.00	0.00
PHE26	H	0.96	0.000	1.00	0.00

**3.25.12 Detailed Probabilities of LYS25HD2:**

Overall probability: 1.000

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS25	1.00	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	0.000	1.00	0.00
LYS25	HB2	1.00	0.000	1.00	0.00
LYS25	HB3	1.00	0.000	1.00	0.00
LYS25	HG2	1.00	0.000	1.00	0.00
LYS25	HG3	1.00	0.000	1.00	0.00
LYS25	HD2	1.00	0.000	1.00	0.00
LYS25	HE2	1.00	0.000	1.00	0.00
LYS25	HE3	1.00	0.000	1.00	0.00
LYS25	H	0.87	0.000	1.00	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	0.000	1.00	0.00
LYS25	HB3	0.99	0.000	1.00	0.00
LYS25	HG2	1.00	0.000	1.00	0.00
LYS25	HG3	1.00	0.000	1.00	0.00
LYS25	HD2	1.00	0.000	1.00	0.00
LYS25	HE2	1.00	0.000	1.00	0.00
LYS25	HE3	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
LYS25	HB3	0.99	0.000	1.00	0.00
LYS25	HG2	1.00	0.000	1.00	0.00
LYS25	HG3	1.00	0.000	1.00	0.00
LYS25	HD2	1.00	0.000	1.00	0.00
LYS25	HE2	1.00	0.000	1.00	0.00
LYS25	HE3	1.00	0.000	1.00	0.00

**3.25.15 Detailed Probabilities of LYS25H:**

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
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	0.00
LEU24	HB2	1.00	0.000	1.00	0.00
LEU24	HB3	1.00	0.000	1.00	0.00
LEU24	HG	0.98	0.000	1.00	0.00
LEU24	H	1.00	0.000	1.00	0.00
LEU24	HD11	0.52	0.000	1.00	0.00
LEU24	HD21	0.59	0.000	1.00	0.00
LYS25	HA	1.00	0.000	1.00	0.00
LYS25	HB2	1.00	0.000	1.00	0.00
LYS25	HB3	1.00	0.000	1.00	0.00
LYS25	HG2	1.00	0.000	1.00	0.00
LYS25	HG3	1.00	0.000	1.00	0.00
LYS25	H	1.00	0.000	1.00	0.00
LYS25	HD2	0.88	0.000	1.00	0.00
PHE26	H	1.00	0.000	1.00	0.00

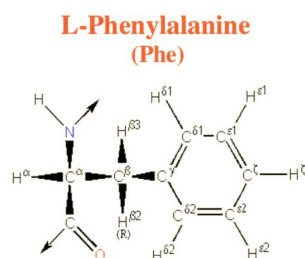
**3.26 PHE(26)**

Figure 16: Image from the BMRB

Residue probability: 0.906

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	0.889	1.000
CB 3.26.2	40.191	40.078	3.616	0.750	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	0.940	1.000
HA 3.26.9	4.835	4.625	1.237	0.923	1.000
HB2 3.26.10	2.442	2.980	0.399	0.875	1.000
HB3 3.26.11	3.160	2.916	0.434	0.875	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	0.715	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	0.717	1.000

**3.26.1 Detailed Probabilities of PHE26CA:**

Overall probability: 0.889

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS25	1.00	1.00
PHE26	1.00	1.00
ILE27	0.50	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	0.012	1.00	0.00
PHE26	HA	1.00	0.000	1.00	0.00
PHE26	HB2	1.00	0.000	1.00	0.00
PHE26	HB3	1.00	0.000	1.00	0.00
PHE26	HD1	1.00	0.005	1.00	0.00
PHE26	HD2	1.00	0.005	1.00	0.00
PHE26	H	1.00	0.000	1.00	0.00
ILE27	HA	1.00	0.141	0.00	0.00
ILE27	H	1.00	0.000	1.00	0.00

**3.26.2 Detailed Probabilities of PHE26CB:**

Overall probability: 0.750

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE26	0.86	1.00
ILE27	0.00	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**

## 3.26 PHE(26)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE26	HA	1.00	0.000	1.00	0.00
PHE26	HB2	1.00	0.000	1.00	0.00
PHE26	HB3	1.00	0.000	1.00	0.00
PHE26	HD1	1.00	0.005	1.00	0.00
PHE26	HD2	1.00	0.005	1.00	0.00
PHE26	HE2	1.00	0.333	0.00	0.00
PHE26	H	1.00	0.000	1.00	0.00
ILE27	H	1.00	0.101	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	0.000	1.00	0.00
PHE26	HB2	1.00	0.000	1.00	0.00
PHE26	HB3	1.00	0.000	1.00	0.00
PHE26	HD1	1.00	0.003	1.00	0.00
PHE26	HD2	1.00	0.003	1.00	0.00
PHE26	HE1	1.00	0.000	1.00	0.00
PHE26	HE2	1.00	0.000	1.00	0.00
PHE26	HZ	1.00	0.001	1.00	0.00
PHE26	H	1.00	0.007	1.00	0.00

## 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	0.000	1.00	0.00
PHE26	HB2	1.00	0.000	1.00	0.00
PHE26	HB3	1.00	0.000	1.00	0.00
PHE26	HD1	1.00	0.003	1.00	0.00
PHE26	HD2	1.00	0.003	1.00	0.00
PHE26	HE1	1.00	0.000	1.00	0.00
PHE26	HE2	1.00	0.000	1.00	0.00
PHE26	HZ	1.00	0.001	1.00	0.00
PHE26	H	0.99	0.000	1.00	0.00

**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	0.00
PHE26	HD2	1.00	0.004	1.00	0.00
PHE26	HE1	1.00	0.000	1.00	0.00
PHE26	HE2	1.00	0.000	1.00	0.00
PHE26	HZ	1.00	0.001	1.00	0.00
PHE26	HA	0.74	0.014	1.00	0.00

**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	0.133	0.00	0.00
PHE26	HB3	1.00	0.647	0.00	0.00
PHE26	HD1	1.00	0.004	1.00	0.00
PHE26	HD2	1.00	0.004	1.00	0.00
PHE26	HE1	1.00	0.000	1.00	0.00
PHE26	HE2	1.00	0.000	1.00	0.00
PHE26	HZ	1.00	0.001	1.00	0.00

**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	0.004	1.00	0.00
PHE26	HD2	1.00	0.004	1.00	0.00
PHE26	HE1	1.00	0.000	1.00	0.00
PHE26	HE2	1.00	0.000	1.00	0.00
PHE26	HZ	1.00	0.001	1.00	0.00

**3.26.8 Detailed Probabilities of PHE26N:**

Overall probability: 0.940

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS25	1.00	1.00
PHE26	1.00	1.00
ILE27	0.68	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	0.000	1.00	0.00
LYS25	HB2	1.00	0.000	1.00	0.00
LYS25	HB3	1.00	0.000	1.00	0.00
LYS25	HG2	0.98	0.000	1.00	0.00
LYS25	HG3	0.96	0.000	1.00	0.00
LYS25	H	1.00	0.000	1.00	0.00
LYS25	HD2	0.54	0.000	1.00	0.00
PHE26	HA	1.00	0.000	1.00	0.00
PHE26	HB2	1.00	0.000	1.00	0.00
PHE26	HB3	1.00	0.000	1.00	0.00
PHE26	HD1	1.00	0.005	1.00	0.00
PHE26	HD2	0.99	0.005	1.00	0.00
PHE26	H	1.00	0.000	1.00	0.00
ILE27	HA	0.96	0.141	0.04	0.00
ILE27	H	1.00	0.000	1.00	0.00
ILE27	HG13	0.53	0.022	1.00	0.00

**3.26.9 Detailed Probabilities of PHE26HA:**

Overall probability: 0.923

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS25	1.00	1.00
PHE26	1.00	1.00
ILE27	0.50	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	0.012	1.00	0.00
LYS25	HB2	0.65	0.012	1.00	0.00
LYS25	HB3	0.87	0.012	1.00	0.00
LYS25	H	0.92	0.012	1.00	0.00
PHE26	HA	1.00	0.000	1.00	0.00
PHE26	HB2	1.00	0.000	1.00	0.00
PHE26	HB3	1.00	0.000	1.00	0.00
PHE26	HD1	1.00	0.000	1.00	0.00
PHE26	HD2	1.00	0.000	1.00	0.00
PHE26	H	1.00	0.000	1.00	0.00
PHE26	HE1	0.74	0.014	1.00	0.00
ILE27	HA	1.00	0.141	0.00	0.00
ILE27	H	1.00	0.000	1.00	0.00

**3.26.10 Detailed Probabilities of PHE26HB2:**

Overall probability: 0.875

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
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	0.000	1.00	0.00
PHE26	HB2	1.00	0.000	1.00	0.00
PHE26	HB3	1.00	0.000	1.00	0.00
PHE26	HD1	1.00	0.000	1.00	0.00
PHE26	HD2	1.00	0.000	1.00	0.00
PHE26	HE2	1.00	0.133	0.00	0.00
PHE26	H	1.00	0.000	1.00	0.00
ILE27	H	1.00	0.000	1.00	0.00

**3.26.11 Detailed Probabilities of PHE26HB3:**

Overall probability: 0.875

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	0.000	1.00	0.00
PHE26	HB2	1.00	0.000	1.00	0.00
PHE26	HB3	1.00	0.000	1.00	0.00
PHE26	HD1	1.00	0.000	1.00	0.00
PHE26	HD2	1.00	0.000	1.00	0.00
PHE26	HE2	1.00	0.647	0.00	0.00
PHE26	H	1.00	0.000	1.00	0.00
ILE27	H	1.00	0.000	1.00	0.00

**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	0.005	1.00	0.00
PHE26	HB2	1.00	0.005	1.00	0.00
PHE26	HB3	1.00	0.005	1.00	0.00
PHE26	HD1	1.00	0.003	1.00	0.00
PHE26	HD2	1.00	0.003	1.00	0.00
PHE26	HE1	1.00	0.004	1.00	0.00
PHE26	HE2	1.00	0.004	1.00	0.00
PHE26	HZ	1.00	0.004	1.00	0.00
PHE26	H	1.00	0.005	1.00	0.00

**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	0.005	1.00	0.00
PHE26	HB2	1.00	0.005	1.00	0.00
PHE26	HB3	1.00	0.005	1.00	0.00
PHE26	HD1	1.00	0.003	1.00	0.00
PHE26	HD2	1.00	0.003	1.00	0.00
PHE26	HE1	1.00	0.004	1.00	0.00
PHE26	HE2	1.00	0.004	1.00	0.00
PHE26	HZ	1.00	0.004	1.00	0.00
PHE26	H	0.99	0.005	1.00	0.00

**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	0.000	1.00	0.00
PHE26	HD2	1.00	0.000	1.00	0.00
PHE26	HE1	1.00	0.000	1.00	0.00
PHE26	HE2	1.00	0.000	1.00	0.00
PHE26	HZ	1.00	0.000	1.00	0.00

**3.26.15 Detailed Probabilities of PHE26HE2:**

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	0.333	0.00	0.00
PHE26	HB3	1.00	0.333	0.00	0.00
PHE26	HD1	1.00	0.000	1.00	0.00
PHE26	HD2	1.00	0.000	1.00	0.00
PHE26	HE1	1.00	0.000	1.00	0.00
PHE26	HE2	1.00	0.000	1.00	0.00
PHE26	HZ	1.00	0.000	1.00	0.00

**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	0.001	1.00	0.00
PHE26	HD2	1.00	0.001	1.00	0.00
PHE26	HE1	1.00	0.001	1.00	0.00
PHE26	HE2	1.00	0.001	1.00	0.00
PHE26	HZ	1.00	0.001	1.00	0.00

**3.26.17 Detailed Probabilities of PHE26H:**

Overall probability: 0.717

Overall confidence: 1.000

**Inter- and intra-residue probability**

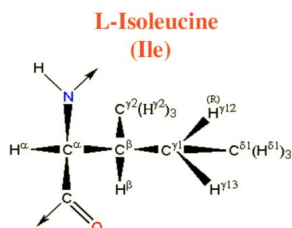
Residue	Probability	Confidence
LYS25	0.67	1.00
PHE26	1.00	1.00
ILE27	0.02	1.00

**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	1.571	0.00	0.00
LYS25	HB2	1.00	0.000	1.00	0.00
LYS25	HB3	1.00	0.000	1.00	0.00
LYS25	HG2	0.98	0.000	1.00	0.00
LYS25	HG3	0.96	0.000	1.00	0.00
LYS25	H	1.00	0.849	0.00	0.00
PHE26	HA	1.00	0.000	1.00	0.00
PHE26	HB2	1.00	0.000	1.00	0.00
PHE26	HB3	1.00	0.000	1.00	0.00
PHE26	HD1	1.00	0.007	1.00	0.00
PHE26	HD2	0.99	0.000	1.00	0.00
PHE26	H	1.00	0.000	1.00	0.00
ILE27	HA	0.96	4.935	0.04	0.00
ILE27	H	1.00	0.328	0.00	0.00



Residue probability: 0.885  
Residue probability confidence: 1.000

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	0.670	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	1.000	1.000
CG2 3.27.4	17.678	17.574	1.928	1.000	1.000
CD1 3.27.5	13.986	13.545	3.646	1.000	1.000
N 3.27.6	124.997	121.467	6.098	0.801	1.000
HA 3.27.7	4.694	4.185	1.403	0.754	1.000
HB 3.27.8	1.813	1.776	0.310	0.889	1.000
HG12 3.27.9	0.970	1.271	0.411	1.000	1.000
HG13 3.27.10	1.237	1.186	0.426	1.000	1.000
HG2 3.27.11	0.918	0.762	0.283	1.000	1.000
HD1 3.27.12	0.665	0.668	0.293	1.000	1.000
H 3.27.13	9.301	8.301	0.685	0.617	1.000

Overall probability: 0.670  
Overall confidence: 1.000

Residue	Probability	Confidence
PHE26	0.02	1.00
ILE27	0.86	1.00
PRO28	0.67	1.00

## Residues TOC

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	0.141	0.00	0.00
PHE26	H	0.96	4.935	0.04	0.00
ILE27	HA	1.00	0.000	1.00	0.00
ILE27	HB	1.00	0.000	1.00	0.00
ILE27	HG12	1.00	0.000	1.00	0.00
ILE27	HG13	1.00	0.000	1.00	0.00
ILE27	HG21	1.00	0.000	1.00	0.00
ILE27	HD11	0.97	0.000	1.00	0.00
ILE27	H	1.00	4.607	0.00	0.00
PRO28	HA	1.00	0.170	0.00	0.00
PRO28	HD2	1.00	0.007	1.00	0.00
PRO28	HD3	1.00	0.004	1.00	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	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	0.000	1.00	0.00
ILE27	HB	1.00	0.000	1.00	0.00
ILE27	HG12	1.00	0.000	1.00	0.00
ILE27	HG13	1.00	0.000	1.00	0.00
ILE27	HG21	1.00	0.000	1.00	0.00
ILE27	HD11	1.00	0.000	1.00	0.00
ILE27	H	1.00	0.000	1.00	0.00
PRO28	HD2	0.99	0.822	0.01	0.00
PRO28	HD3	1.00	0.560	0.00	0.00

**3.27.3 Detailed Probabilities of ILE27CG1:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE27	1.00	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	0.000	1.00	0.00
ILE27	HB	1.00	0.000	1.00	0.00
ILE27	HG12	1.00	0.000	1.00	0.00
ILE27	HG13	1.00	0.000	1.00	0.00
ILE27	HG21	1.00	0.000	1.00	0.00
ILE27	HD11	1.00	0.000	1.00	0.00
ILE27	H	1.00	0.000	1.00	0.00

**3.27.4 Detailed Probabilities of ILE27CG2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE27	1.00	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	0.000	1.00	0.00
ILE27	HB	1.00	0.000	1.00	0.00
ILE27	HG12	1.00	0.000	1.00	0.00
ILE27	HG13	1.00	0.000	1.00	0.00
ILE27	HG21	1.00	0.000	1.00	0.00
ILE27	HD11	0.99	0.000	1.00	0.00
ILE27	H	1.00	0.000	1.00	0.00

**3.27.5 Detailed Probabilities of ILE27CD1:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE27	1.00	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	0.000	1.00	0.00
ILE27	HB	1.00	0.000	1.00	0.00
ILE27	HG12	1.00	0.000	1.00	0.00
ILE27	HG13	1.00	0.000	1.00	0.00
ILE27	HG21	0.99	0.000	1.00	0.00
ILE27	HD11	1.00	0.000	1.00	0.00
ILE27	H	0.94	0.000	1.00	0.00

**3.27.6 Detailed Probabilities of ILE27N:**

Overall probability: 0.801

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE26	0.83	1.00
ILE27	1.00	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	0.000	1.00	0.00
PHE26	HB2	1.00	0.000	1.00	0.00
PHE26	HB3	1.00	0.000	1.00	0.00
PHE26	H	1.00	0.328	0.00	0.00
PHE26	HD1	0.77	0.005	1.00	0.00
PHE26	HD2	0.64	0.005	1.00	0.00
ILE27	HA	1.00	0.000	1.00	0.00
ILE27	HB	1.00	0.000	1.00	0.00
ILE27	HG12	1.00	0.000	1.00	0.00
ILE27	HG13	1.00	0.000	1.00	0.00
ILE27	HG21	1.00	0.000	1.00	0.00
ILE27	H	1.00	0.000	1.00	0.00
ILE27	HD11	0.94	0.000	1.00	0.00
PRO28	HD2	0.99	0.712	0.01	0.00
PRO28	HD3	0.99	0.560	0.01	0.00

**3.27.7 Detailed Probabilities of ILE27HA:**

Overall probability: 0.754

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE26	0.02	1.00
ILE27	1.00	1.00
PRO28	0.67	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	0.141	0.00	0.00
PHE26	H	0.96	0.141	0.04	0.00
ILE27	HA	1.00	0.000	1.00	0.00
ILE27	HB	1.00	0.000	1.00	0.00
ILE27	HG12	1.00	0.000	1.00	0.00
ILE27	HG13	1.00	0.000	1.00	0.00
ILE27	HG21	1.00	0.000	1.00	0.00
ILE27	HD11	0.97	0.000	1.00	0.00
ILE27	H	1.00	0.000	1.00	0.00
PRO28	HA	1.00	0.170	0.00	0.00
PRO28	HD2	1.00	0.011	1.00	0.00
PRO28	HD3	1.00	0.001	1.00	0.00

**3.27.8 Detailed Probabilities of ILE27HB:**

Overall probability: 0.889

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE27	1.00	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	0.000	1.00	0.00
ILE27	HB	1.00	0.000	1.00	0.00
ILE27	HG12	1.00	0.000	1.00	0.00
ILE27	HG13	1.00	0.000	1.00	0.00
ILE27	HG21	1.00	0.000	1.00	0.00
ILE27	HD11	1.00	0.000	1.00	0.00
ILE27	H	1.00	0.000	1.00	0.00
PRO28	HD2	0.99	0.018	1.00	0.00
PRO28	HD3	1.00	0.062	0.00	0.00

**3.27.9 Detailed Probabilities of ILE27HG12:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE27	1.00	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	0.000	1.00	0.00
ILE27	HB	1.00	0.000	1.00	0.00
ILE27	HG12	1.00	0.000	1.00	0.00
ILE27	HG13	1.00	0.000	1.00	0.00
ILE27	HG21	1.00	0.000	1.00	0.00
ILE27	HD11	1.00	0.000	1.00	0.00
ILE27	H	1.00	0.000	1.00	0.00

**3.27.10 Detailed Probabilities of ILE27HG13:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE27	1.00	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	0.000	1.00	0.00
ILE27	HB	1.00	0.000	1.00	0.00
ILE27	HG12	1.00	0.000	1.00	0.00
ILE27	HG13	1.00	0.000	1.00	0.00
ILE27	HG21	1.00	0.000	1.00	0.00
ILE27	HD11	1.00	0.000	1.00	0.00
ILE27	H	1.00	0.000	1.00	0.00

**3.27.11 Detailed Probabilities of ILE27HG21:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE27	1.00	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	0.000	1.00	0.00
ILE27	HB	1.00	0.000	1.00	0.00
ILE27	HG12	1.00	0.000	1.00	0.00
ILE27	HG13	1.00	0.000	1.00	0.00
ILE27	HG21	1.00	0.000	1.00	0.00
ILE27	HD11	0.99	0.000	1.00	0.00
ILE27	H	1.00	0.000	1.00	0.00

**3.27.12 Detailed Probabilities of ILE27HD11:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE27	1.00	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	0.000	1.00	0.00
ILE27	HB	1.00	0.000	1.00	0.00
ILE27	HG12	1.00	0.000	1.00	0.00
ILE27	HG13	1.00	0.000	1.00	0.00
ILE27	HG21	0.99	0.000	1.00	0.00
ILE27	HD11	1.00	0.000	1.00	0.00
ILE27	H	0.94	0.000	1.00	0.00

**3.27.13 Detailed Probabilities of ILE27H:**

Overall probability: 0.617

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE26	0.50	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	0.000	1.00	0.00
PHE26	HB2	1.00	0.101	0.00	0.00
PHE26	HB3	1.00	0.328	0.00	0.00
PHE26	H	1.00	0.000	1.00	0.00
ILE27	HA	1.00	4.607	0.00	0.00
ILE27	HB	1.00	0.000	1.00	0.00
ILE27	HG12	1.00	0.000	1.00	0.00
ILE27	HG13	1.00	0.000	1.00	0.00
ILE27	HG21	1.00	0.000	1.00	0.00
ILE27	H	1.00	0.000	1.00	0.00
ILE27	HD11	0.94	0.000	1.00	0.00
PRO28	HD2	0.99	0.110	0.01	0.00
PRO28	HD3	0.99	0.105	0.01	0.00

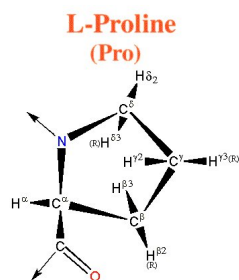
**3.28 PRO(28)**

Figure 18: Image from the BMRB

**Residue probability:** 0.872**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	0.636	1.000
CB 3.28.2	32.443	33.632	13.629	1.000	1.000
CG 3.28.3	26.610	28.412	13.801	1.000	1.000
CD 3.28.4	50.627	49.797	3.175	0.917	1.000
N	NA	—	—	0.000	0.000
HA 3.28.5	4.524	4.332	0.427	0.636	1.000
HB2 3.28.6	1.751	2.099	0.501	0.809	1.000
HB3 3.28.7	1.640	2.052	0.596	1.000	1.000
HG2 3.28.8	1.944	1.927	0.364	1.000	1.000
HG3 3.28.9	1.499	1.907	0.417	1.000	1.000
HD2 3.28.10	3.872	3.640	0.682	0.770	1.000
HD3 3.28.11	4.134	3.558	0.522	0.819	1.000

**3.28.1 Detailed Probabilities of PRO28CA:****Overall probability:** 0.636**Overall confidence:** 1.000**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE27	0.00	1.00
PRO28	0.86	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	0.170	0.00	0.00
PRO28	HA	1.00	0.000	1.00	0.00
PRO28	HB2	1.00	0.000	1.00	0.00
PRO28	HB3	1.00	0.000	1.00	0.00
PRO28	HG2	1.00	0.000	1.00	0.00
PRO28	HG3	1.00	0.000	1.00	0.00
PRO28	HD2	1.00	0.287	0.00	0.00
PRO28	HD3	1.00	0.025	1.00	0.00
GLY29	HA2	1.00	0.517	0.00	0.00
GLY29	HA3	1.00	0.133	0.00	0.00
GLY29	H	1.00	0.000	1.00	0.00

**3.28.2 Detailed Probabilities of PRO28CB:**

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

**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**

## 3.28 PRO(28)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PRO28	HA	1.00	0.000	1.00	0.00
PRO28	HB2	1.00	0.000	1.00	0.00
PRO28	HB3	1.00	0.000	1.00	0.00
PRO28	HG2	1.00	0.000	1.00	0.00
PRO28	HG3	1.00	0.000	1.00	0.00
PRO28	HD2	1.00	0.000	1.00	0.00
PRO28	HD3	1.00	0.000	1.00	0.00
GLY29	H	1.00	0.000	1.00	0.00

## 3.28.3 Detailed Probabilities of PRO28CG:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
PRO28	1.00	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	0.00
PRO28	HB2	1.00	0.000	1.00	0.00
PRO28	HB3	1.00	0.000	1.00	0.00
PRO28	HG2	1.00	0.000	1.00	0.00
PRO28	HG3	1.00	0.000	1.00	0.00
PRO28	HD2	1.00	0.000	1.00	0.00
PRO28	HD3	1.00	0.000	1.00	0.00

## 3.28.4 Detailed Probabilities of PRO28CD:

Overall probability: 0.917

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
ILE27	0.80	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	0.011	1.00	0.00
ILE27	HB	0.99	0.018	1.00	0.00
ILE27	H	0.99	0.110	0.01	0.00
ILE27	HG12	0.86	0.008	1.00	0.00
ILE27	HG21	0.95	0.010	1.00	0.00
PRO28	HA	1.00	0.019	1.00	0.00
PRO28	HB2	1.00	0.000	1.00	0.00
PRO28	HB3	1.00	0.000	1.00	0.00
PRO28	HG2	1.00	0.000	1.00	0.00
PRO28	HG3	1.00	0.000	1.00	0.00
PRO28	HD2	1.00	0.000	1.00	0.00
PRO28	HD3	1.00	0.000	1.00	0.00

**3.28.5 Detailed Probabilities of PRO28HA:**

Overall probability: 0.636

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE27	0.00	1.00
PRO28	0.86	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	0.170	0.00	0.00
PRO28	HA	1.00	0.000	1.00	0.00
PRO28	HB2	1.00	0.000	1.00	0.00
PRO28	HB3	1.00	0.000	1.00	0.00
PRO28	HG2	1.00	0.000	1.00	0.00
PRO28	HG3	1.00	0.000	1.00	0.00
PRO28	HD2	1.00	0.019	1.00	0.00
PRO28	HD3	1.00	0.169	0.00	0.00
GLY29	HA2	1.00	0.498	0.00	0.00
GLY29	HA3	1.00	0.498	0.00	0.00
GLY29	H	1.00	0.000	1.00	0.00

**3.28.6 Detailed Probabilities of PRO28HB2:**

Overall probability: 0.809

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO28	1.00	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	0.000	1.00	0.00
PRO28	HB2	1.00	0.000	1.00	0.00
PRO28	HB3	1.00	0.000	1.00	0.00
PRO28	HG2	1.00	0.000	1.00	0.00
PRO28	HG3	1.00	0.000	1.00	0.00
PRO28	HD2	1.00	0.000	1.00	0.00
PRO28	HD3	1.00	0.000	1.00	0.00
GLY29	HA2	0.95	0.835	0.05	0.00
GLY29	HA3	0.95	0.828	0.05	0.00
GLY29	H	1.00	0.013	1.00	0.00

**3.28.7 Detailed Probabilities of PRO28HB3:**

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

**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	0.000	1.00	0.00
PRO28	HB2	1.00	0.000	1.00	0.00
PRO28	HB3	1.00	0.000	1.00	0.00
PRO28	HG2	1.00	0.000	1.00	0.00
PRO28	HG3	1.00	0.000	1.00	0.00
PRO28	HD2	1.00	0.000	1.00	0.00
PRO28	HD3	1.00	0.000	1.00	0.00
GLY29	H	1.00	0.006	1.00	0.00

**3.28.8 Detailed Probabilities of PRO28HG2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO28	1.00	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	0.00
PRO28	HB2	1.00	0.000	1.00	0.00
PRO28	HB3	1.00	0.000	1.00	0.00
PRO28	HG2	1.00	0.000	1.00	0.00
PRO28	HG3	1.00	0.000	1.00	0.00
PRO28	HD2	1.00	0.000	1.00	0.00
PRO28	HD3	1.00	0.000	1.00	0.00

**3.28.9 Detailed Probabilities of PRO28HG3:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO28	1.00	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	0.000	1.00	0.00
PRO28	HB2	1.00	0.000	1.00	0.00
PRO28	HB3	1.00	0.000	1.00	0.00
PRO28	HG2	1.00	0.000	1.00	0.00
PRO28	HG3	1.00	0.000	1.00	0.00
PRO28	HD2	1.00	0.000	1.00	0.00
PRO28	HD3	1.00	0.000	1.00	0.00

**3.28.10 Detailed Probabilities of PRO28HD2:**

Overall probability: 0.770

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE27	0.67	1.00
PRO28	0.86	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	0.007	1.00	0.00
ILE27	HB	0.99	0.822	0.01	0.00
ILE27	H	0.99	0.712	0.01	0.00
ILE27	HG12	0.86	0.016	1.00	0.00
ILE27	HG13	0.86	0.024	1.00	0.00
ILE27	HG21	0.95	0.012	1.00	0.00
PRO28	HA	1.00	0.287	0.00	0.00
PRO28	HB2	1.00	0.000	1.00	0.00
PRO28	HB3	1.00	0.000	1.00	0.00
PRO28	HG2	1.00	0.000	1.00	0.00
PRO28	HG3	1.00	0.000	1.00	0.00
PRO28	HD2	1.00	0.000	1.00	0.00
PRO28	HD3	1.00	0.000	1.00	0.00

**3.28.11 Detailed Probabilities of PRO28HD3:**

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	0.004	1.00	0.00
ILE27	HB	1.00	0.560	0.00	0.00
ILE27	H	0.99	0.560	0.01	0.00
ILE27	HG21	0.84	0.022	1.00	0.00
PRO28	HA	1.00	0.025	1.00	0.00
PRO28	HB2	1.00	0.000	1.00	0.00
PRO28	HB3	1.00	0.000	1.00	0.00
PRO28	HG2	1.00	0.000	1.00	0.00
PRO28	HG3	1.00	0.000	1.00	0.00
PRO28	HD2	1.00	0.000	1.00	0.00
PRO28	HD3	1.00	0.000	1.00	0.00

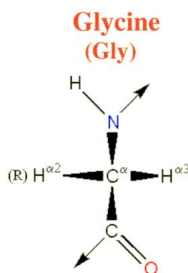
**3.29 GLY(29)**

Figure 19: 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	172.714	173.872	2.493	0.000	0.000
CA 3.29.1	45.432	45.581	4.381	0.578	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	0.578	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	0.889	1.000

**3.29.1 Detailed Probabilities of GLY29CA:**

Overall probability: 0.578

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO28	0.02	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**

## 3.29 GLY(29)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PRO28	HA	1.00	0.498	0.00	0.00
PRO28	HB2	0.95	0.835	0.05	0.00
GLY29	HA2	1.00	0.000	1.00	0.00
GLY29	HA3	1.00	0.000	1.00	0.00
GLY29	H	1.00	0.000	1.00	0.00
LYS30	HA	1.00	0.627	0.00	0.00
LYS30	H	1.00	0.000	1.00	0.00

## 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	0.00
PRO28	HB2	1.00	0.013	1.00	0.00
PRO28	HB3	1.00	0.006	1.00	0.00
PRO28	HG2	0.88	0.001	1.00	0.00
PRO28	HD3	0.62	0.000	1.00	0.00
GLY29	HA2	1.00	0.000	1.00	0.00
GLY29	HA3	1.00	0.000	1.00	0.00
GLY29	H	1.00	0.000	1.00	0.00
LYS30	H	1.00	0.000	1.00	0.00
LYS30	HB2	0.61	0.018	1.00	0.00

## 3.29.3 Detailed Probabilities of GLY29HA2:

Overall probability: 0.578

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO28	0.02	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	0.517	0.00	0.00
PRO28	HB2	0.95	0.230	0.05	0.00
GLY29	HA2	1.00	0.000	1.00	0.00
GLY29	HA3	1.00	0.000	1.00	0.00
GLY29	H	1.00	0.000	1.00	0.00
LYS30	HA	1.00	0.084	0.00	0.00
LYS30	H	1.00	0.000	1.00	0.00

**3.29.4 Detailed Probabilities of GLY29HA3:**

Overall probability: 0.578

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO28	0.02	1.00
GLY29	1.00	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	0.133	0.00	0.00
PRO28	HB2	0.95	0.108	0.05	0.00
GLY29	HA2	1.00	0.000	1.00	0.00
GLY29	HA3	1.00	0.000	1.00	0.00
GLY29	H	1.00	0.000	1.00	0.00
LYS30	HA	1.00	0.260	0.00	0.00
LYS30	H	1.00	0.000	1.00	0.00

## 3.29.5 Detailed Probabilities of GLY29H:

Overall probability: 0.889

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
PRO28	0.80	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	0.00
PRO28	HB2	1.00	0.387	0.00	0.00
PRO28	HB3	1.00	0.000	1.00	0.00
PRO28	HG2	0.88	0.000	1.00	0.00
PRO28	HD3	0.62	0.000	1.00	0.00
GLY29	HA2	1.00	0.000	1.00	0.00
GLY29	HA3	1.00	0.000	1.00	0.00
GLY29	H	1.00	0.000	1.00	0.00
LYS30	H	1.00	0.000	1.00	0.00

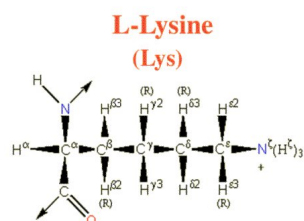


Figure 20: Image from the BMRB

Residue probability: 0.948  
 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	0.769	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	1.000	0.875
N 3.30.6	117.771	120.954	4.210	0.835	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	1.000	1.000
HB3 3.30.9	1.016	1.742	0.385	1.000	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	1.000	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	1.000	0.875
H 3.30.15	6.801	8.185	0.605	0.820	1.000
HZ	NA	—	—	0.000	0.000

**3.30.1 Detailed Probabilities of LYS30CA:**

Overall probability: 0.769  
 Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLY29	0.00	1.00
LYS30	1.00	1.00
PRO31	0.67	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	0.084	0.00	0.00
GLY29	HA3	1.00	0.260	0.00	0.00
LYS30	HA	1.00	0.000	1.00	0.00
LYS30	HB2	1.00	0.000	1.00	0.00
LYS30	HB3	1.00	0.000	1.00	0.00
LYS30	HG2	1.00	0.000	1.00	0.00
LYS30	HG3	1.00	0.000	1.00	0.00
LYS30	HD2	0.98	0.000	1.00	0.00
LYS30	HD3	0.98	0.000	1.00	0.00
LYS30	H	1.00	0.000	1.00	0.00
PRO31	HA	1.00	0.317	0.00	0.00
PRO31	HD2	1.00	0.004	1.00	0.00
PRO31	HD3	1.00	0.004	1.00	0.00

**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
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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS30	HA	1.00	0.000	1.00	0.00
LYS30	HB2	1.00	0.000	1.00	0.00
LYS30	HB3	1.00	0.000	1.00	0.00
LYS30	HG2	1.00	0.000	1.00	0.00
LYS30	HG3	1.00	0.000	1.00	0.00
LYS30	HD2	1.00	0.000	1.00	0.00
LYS30	HD3	1.00	0.000	1.00	0.00
LYS30	HE2	0.98	0.000	1.00	0.00
LYS30	H	1.00	0.000	1.00	0.00
PRO31	HD2	0.99	0.004	1.00	0.00
PRO31	HD3	1.00	0.008	1.00	0.00

**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	0.000	1.00	0.00
LYS30	HB2	1.00	0.000	1.00	0.00
LYS30	HB3	1.00	0.000	1.00	0.00
LYS30	HG2	1.00	0.000	1.00	0.00
LYS30	HG3	1.00	0.000	1.00	0.00
LYS30	HD2	1.00	0.000	1.00	0.00
LYS30	HD3	1.00	0.000	1.00	0.00
LYS30	HE2	1.00	0.000	1.00	0.00
LYS30	H	1.00	0.000	1.00	0.00

**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	0.00
LYS30	HB2	1.00	0.000	1.00	0.00
LYS30	HB3	1.00	0.000	1.00	0.00
LYS30	HG2	1.00	0.000	1.00	0.00
LYS30	HG3	1.00	0.000	1.00	0.00
LYS30	HD2	1.00	0.000	1.00	0.00
LYS30	HD3	1.00	0.000	1.00	0.00
LYS30	HE2	1.00	0.000	1.00	0.00

**3.30.5 Detailed Probabilities of LYS30CE:**

Overall probability: 1.000

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS30	1.00	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	0.00
LYS30	HB3	0.99	0.000	1.00	0.00
LYS30	HG2	1.00	0.000	1.00	0.00
LYS30	HG3	1.00	0.000	1.00	0.00
LYS30	HD2	1.00	0.000	1.00	0.00
LYS30	HD3	1.00	0.000	1.00	0.00
LYS30	HE2	1.00	0.000	1.00	0.00

**3.30.6 Detailed Probabilities of LYS30N:**

Overall probability: 0.835

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLY29	1.00	1.00
LYS30	1.00	1.00
PRO31	0.01	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	0.000	1.00	0.00
GLY29	HA3	1.00	0.000	1.00	0.00
GLY29	H	1.00	0.000	1.00	0.00
LYS30	HA	1.00	0.000	1.00	0.00
LYS30	HB2	1.00	0.000	1.00	0.00
LYS30	HB3	1.00	0.000	1.00	0.00
LYS30	HG2	1.00	0.000	1.00	0.00
LYS30	HG3	1.00	0.000	1.00	0.00
LYS30	H	1.00	0.000	1.00	0.00
LYS30	HD3	0.87	0.000	1.00	0.00
PRO31	HD2	0.99	0.128	0.01	0.00
PRO31	HD3	0.99	0.080	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	0.00	1.00
LYS30	1.00	1.00
PRO31	0.80	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	0.627	0.00	0.00
GLY29	HA3	1.00	0.627	0.00	0.00
LYS30	HA	1.00	0.000	1.00	0.00
LYS30	HB2	1.00	0.000	1.00	0.00
LYS30	HB3	1.00	0.000	1.00	0.00
LYS30	HG2	1.00	0.000	1.00	0.00
LYS30	HG3	1.00	0.000	1.00	0.00
LYS30	HD2	0.98	0.000	1.00	0.00
LYS30	HD3	0.98	0.000	1.00	0.00
LYS30	H	1.00	0.000	1.00	0.00
PRO31	HA	1.00	0.048	0.00	0.00
PRO31	HD2	1.00	0.003	1.00	0.00
PRO31	HD3	1.00	0.003	1.00	0.00
PRO31	HG2	0.93	0.004	1.00	0.00
PRO31	HG3	0.92	0.013	1.00	0.00

## 3.30.8 Detailed Probabilities of LYS30HB2:

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
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	0.000	1.00	0.00
LYS30	HB2	1.00	0.000	1.00	0.00
LYS30	HB3	1.00	0.000	1.00	0.00
LYS30	HG2	1.00	0.000	1.00	0.00
LYS30	HG3	1.00	0.000	1.00	0.00
LYS30	HD2	1.00	0.000	1.00	0.00
LYS30	HD3	1.00	0.000	1.00	0.00
LYS30	HE2	0.98	0.000	1.00	0.00
LYS30	H	1.00	0.000	1.00	0.00
PRO31	HD2	0.99	0.005	1.00	0.00
PRO31	HD3	1.00	0.002	1.00	0.00

## 3.30.9 Detailed Probabilities of LYS30HB3:

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	0.000	1.00	0.00
LYS30	HB2	1.00	0.000	1.00	0.00
LYS30	HB3	1.00	0.000	1.00	0.00
LYS30	HG2	1.00	0.000	1.00	0.00
LYS30	HG3	1.00	0.000	1.00	0.00
LYS30	HD2	1.00	0.000	1.00	0.00
LYS30	HD3	1.00	0.000	1.00	0.00
LYS30	HE2	0.99	0.000	1.00	0.00
LYS30	H	1.00	0.000	1.00	0.00
PRO31	HD2	0.99	0.010	1.00	0.00
PRO31	HD3	1.00	0.002	1.00	0.00

**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	0.000	1.00	0.00
LYS30	HB2	1.00	0.000	1.00	0.00
LYS30	HB3	1.00	0.000	1.00	0.00
LYS30	HG2	1.00	0.000	1.00	0.00
LYS30	HG3	1.00	0.000	1.00	0.00
LYS30	HD2	1.00	0.000	1.00	0.00
LYS30	HD3	1.00	0.000	1.00	0.00
LYS30	HE2	1.00	0.000	1.00	0.00
LYS30	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
LYS30	HB2	1.00	0.000	1.00	0.00
LYS30	HB3	1.00	0.000	1.00	0.00
LYS30	HG2	1.00	0.000	1.00	0.00
LYS30	HG3	1.00	0.000	1.00	0.00
LYS30	HD2	1.00	0.000	1.00	0.00
LYS30	HD3	1.00	0.000	1.00	0.00
LYS30	HE2	1.00	0.000	1.00	0.00
LYS30	H	1.00	0.000	1.00	0.00

**3.30.12 Detailed Probabilities of LYS30HD2:**

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**

## 3.30 LYS(30)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS30	HA	0.98	0.000	1.00	0.00
LYS30	HB2	1.00	0.000	1.00	0.00
LYS30	HB3	1.00	0.000	1.00	0.00
LYS30	HG2	1.00	0.000	1.00	0.00
LYS30	HG3	1.00	0.000	1.00	0.00
LYS30	HD2	1.00	0.000	1.00	0.00
LYS30	HD3	1.00	0.000	1.00	0.00
LYS30	HE2	1.00	0.000	1.00	0.00

## 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	0.000	1.00	0.00
LYS30	HB2	1.00	0.000	1.00	0.00
LYS30	HB3	1.00	0.000	1.00	0.00
LYS30	HG2	1.00	0.000	1.00	0.00
LYS30	HG3	1.00	0.000	1.00	0.00
LYS30	HD2	1.00	0.000	1.00	0.00
LYS30	HD3	1.00	0.000	1.00	0.00
LYS30	HE2	1.00	0.000	1.00	0.00
LYS30	H	0.87	0.000	1.00	0.00

## 3.30.14 Detailed Probabilities of LYS30HE2:

Overall probability: 1.000

Overall confidence: 0.875

## Inter- and intra-residue probability

Residue	Probability	Confidence
LYS30	1.00	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	0.00
LYS30	HB3	0.99	0.000	1.00	0.00
LYS30	HG2	1.00	0.000	1.00	0.00
LYS30	HG3	1.00	0.000	1.00	0.00
LYS30	HD2	1.00	0.000	1.00	0.00
LYS30	HD3	1.00	0.000	1.00	0.00
LYS30	HE2	1.00	0.000	1.00	0.00

**3.30.15 Detailed Probabilities of LYS30H:**

Overall probability: 0.820

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLY29	1.00	1.00
LYS30	1.00	1.00
PRO31	0.01	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	0.000	1.00	0.00
GLY29	HA3	1.00	0.000	1.00	0.00
GLY29	H	1.00	0.000	1.00	0.00
LYS30	HA	1.00	0.000	1.00	0.00
LYS30	HB2	1.00	0.000	1.00	0.00
LYS30	HB3	1.00	0.000	1.00	0.00
LYS30	HG2	1.00	0.000	1.00	0.00
LYS30	HG3	1.00	0.000	1.00	0.00
LYS30	H	1.00	0.000	1.00	0.00
PRO31	HD2	0.99	0.510	0.01	0.00
PRO31	HD3	0.99	0.510	0.01	0.00

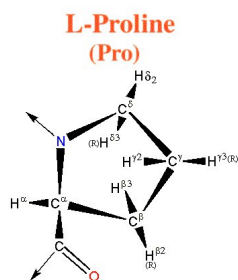


Figure 21: Image from the BMRB

**Residue probability:** 0.935  
**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	1.000	1.000
CG 3.31.3	27.658	28.412	13.801	1.000	1.000
CD 3.31.4	50.171	49.797	3.175	0.929	1.000
N	NA	—	—	0.000	0.000
HA 3.31.5	4.336	4.332	0.427	0.782	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	1.000	1.000
HG2 3.31.8	2.107	1.927	0.364	1.000	1.000
HG3 3.31.9	1.972	1.907	0.417	1.000	1.000
HD2 3.31.10	3.770	3.640	0.682	0.929	1.000
HD3 3.31.11	3.562	3.558	0.522	0.924	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	0.000	1.00	0.00
PRO31	HB2	1.00	0.000	1.00	0.00
PRO31	HB3	1.00	0.000	1.00	0.00
PRO31	HG2	1.00	0.000	1.00	0.00
PRO31	HG3	1.00	0.000	1.00	0.00
PRO31	HD2	1.00	0.000	1.00	0.00
PRO31	HD3	1.00	0.000	1.00	0.00
VAL32	HA	1.00	0.118	0.00	0.00
VAL32	H	1.00	0.000	1.00	0.00
VAL32	HB	0.51	0.003	1.00	0.00
VAL32	HG21	0.54	0.005	1.00	0.00

**3.31.2 Detailed Probabilities of PRO31CB:**

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

**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	0.000	1.00	0.00
PRO31	HB2	1.00	0.000	1.00	0.00
PRO31	HB3	1.00	0.000	1.00	0.00
PRO31	HG2	1.00	0.000	1.00	0.00
PRO31	HG3	1.00	0.000	1.00	0.00
PRO31	HD2	1.00	0.000	1.00	0.00
PRO31	HD3	1.00	0.000	1.00	0.00
VAL32	H	1.00	0.000	1.00	0.00

## 3.31.3 Detailed Probabilities of PRO31CG:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
PRO31	1.00	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	0.000	1.00	0.00
PRO31	HB2	1.00	0.000	1.00	0.00
PRO31	HB3	1.00	0.000	1.00	0.00
PRO31	HG2	1.00	0.000	1.00	0.00
PRO31	HG3	1.00	0.000	1.00	0.00
PRO31	HD2	1.00	0.000	1.00	0.00
PRO31	HD3	1.00	0.000	1.00	0.00

## 3.31.4 Detailed Probabilities of PRO31CD:

Overall probability: 0.929

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
LYS30	0.86	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	0.003	1.00	0.00
LYS30	HB2	0.99	0.005	1.00	0.00
LYS30	HB3	0.99	0.010	1.00	0.00
LYS30	H	0.99	0.510	0.01	0.00
LYS30	HG2	0.93	0.003	1.00	0.00
LYS30	HG3	0.92	0.004	1.00	0.00
LYS30	HD2	0.66	0.011	1.00	0.00
PRO31	HA	1.00	0.025	1.00	0.00
PRO31	HB2	1.00	0.000	1.00	0.00
PRO31	HB3	1.00	0.000	1.00	0.00
PRO31	HG2	1.00	0.000	1.00	0.00
PRO31	HG3	1.00	0.000	1.00	0.00
PRO31	HD2	1.00	0.000	1.00	0.00
PRO31	HD3	1.00	0.000	1.00	0.00

**3.31.5 Detailed Probabilities of PRO31HA:**

Overall probability: 0.782

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS30	0.00	1.00
PRO31	0.94	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	0.317	0.00	0.00
PRO31	HA	1.00	0.000	1.00	0.00
PRO31	HB2	1.00	0.000	1.00	0.00
PRO31	HB3	1.00	0.000	1.00	0.00
PRO31	HG2	1.00	0.000	1.00	0.00
PRO31	HG3	1.00	0.000	1.00	0.00
PRO31	HD2	1.00	0.025	1.00	0.00
PRO31	HD3	1.00	0.034	0.60	0.00
VAL32	HA	1.00	0.118	0.00	0.00
VAL32	H	1.00	0.000	1.00	0.00
VAL32	HG21	0.54	0.017	1.00	0.00

**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	0.000	1.00	0.00
PRO31	HB2	1.00	0.000	1.00	0.00
PRO31	HB3	1.00	0.000	1.00	0.00
PRO31	HG2	1.00	0.000	1.00	0.00
PRO31	HG3	1.00	0.000	1.00	0.00
PRO31	HD2	1.00	0.000	1.00	0.00
PRO31	HD3	1.00	0.000	1.00	0.00
VAL32	HA	0.99	0.218	0.01	0.00
VAL32	H	1.00	0.000	1.00	0.00

## 3.31.7 Detailed Probabilities of PRO31HB3:

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

## 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	0.000	1.00	0.00
PRO31	HB2	1.00	0.000	1.00	0.00
PRO31	HB3	1.00	0.000	1.00	0.00
PRO31	HG2	1.00	0.000	1.00	0.00
PRO31	HG3	1.00	0.000	1.00	0.00
PRO31	HD2	1.00	0.000	1.00	0.00
PRO31	HD3	1.00	0.000	1.00	0.00
VAL32	H	1.00	0.000	1.00	0.00

## 3.31.8 Detailed Probabilities of PRO31HG2:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
PRO31	1.00	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	0.000	1.00	0.00
PRO31	HB2	1.00	0.000	1.00	0.00
PRO31	HB3	1.00	0.000	1.00	0.00
PRO31	HG2	1.00	0.000	1.00	0.00
PRO31	HG3	1.00	0.000	1.00	0.00
PRO31	HD2	1.00	0.000	1.00	0.00
PRO31	HD3	1.00	0.000	1.00	0.00

**3.31.9 Detailed Probabilities of PRO31HG3:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO31	1.00	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	0.00
PRO31	HB2	1.00	0.000	1.00	0.00
PRO31	HB3	1.00	0.000	1.00	0.00
PRO31	HG2	1.00	0.000	1.00	0.00
PRO31	HG3	1.00	0.000	1.00	0.00
PRO31	HD2	1.00	0.000	1.00	0.00
PRO31	HD3	1.00	0.000	1.00	0.00

**3.31.10 Detailed Probabilities of PRO31HD2:**

Overall probability: 0.929

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS30	0.86	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	0.004	1.00	0.00
LYS30	HB2	0.99	0.004	1.00	0.00
LYS30	HB3	0.99	0.012	1.00	0.00
LYS30	H	0.99	0.128	0.01	0.00
LYS30	HG2	0.93	0.008	1.00	0.00
LYS30	HG3	0.92	0.008	1.00	0.00
LYS30	HD3	0.66	0.000	1.00	0.00
PRO31	HA	1.00	0.000	1.00	0.00
PRO31	HB2	1.00	0.000	1.00	0.00
PRO31	HB3	1.00	0.000	1.00	0.00
PRO31	HG2	1.00	0.000	1.00	0.00
PRO31	HG3	1.00	0.000	1.00	0.00
PRO31	HD2	1.00	0.000	1.00	0.00
PRO31	HD3	1.00	0.000	1.00	0.00

**3.31.11 Detailed Probabilities of PRO31HD3:**

Overall probability: 0.924

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS30	0.83	1.00
PRO31	1.00	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	0.004	1.00	0.00
LYS30	HB2	1.00	0.008	1.00	0.00
LYS30	HB3	1.00	0.008	1.00	0.00
LYS30	H	0.99	0.080	0.01	0.00
LYS30	HG2	0.79	0.007	1.00	0.00
LYS30	HG3	0.78	0.007	1.00	0.00
PRO31	HA	1.00	0.000	1.00	0.00
PRO31	HB2	1.00	0.000	1.00	0.00
PRO31	HB3	1.00	0.000	1.00	0.00
PRO31	HG2	1.00	0.000	1.00	0.00
PRO31	HG3	1.00	0.000	1.00	0.00
PRO31	HD2	1.00	0.000	1.00	0.00
PRO31	HD3	1.00	0.000	1.00	0.00

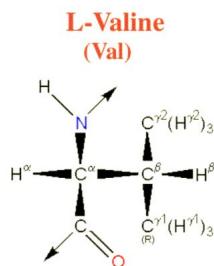
**3.32 VAL(32)**

Figure 22: Image from the BMRB

Residue probability: 0.943

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	1.000	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	0.730	1.000
HB 3.32.7	2.110	1.980	0.322	1.000	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	0.218	0.01	0.00
PRO31	HG2	0.65	0.003	1.00	0.00
VAL32	HA	1.00	0.000	1.00	0.00
VAL32	HB	1.00	0.000	1.00	0.00
VAL32	HG11	1.00	0.000	1.00	0.00
VAL32	HG21	1.00	0.000	1.00	0.00
VAL32	H	1.00	0.000	1.00	0.00
LEU33	HA	1.00	0.417	0.00	0.00
LEU33	H	1.00	0.000	1.00	0.00

**3.32.2 Detailed Probabilities of VAL32CB:**

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
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	0.000	1.00	0.00
VAL32	HB	1.00	0.000	1.00	0.00
VAL32	HG11	1.00	0.000	1.00	0.00
VAL32	HG21	1.00	0.000	1.00	0.00
VAL32	H	1.00	0.000	1.00	0.00
LEU33	H	1.00	0.000	1.00	0.00

**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	0.00
VAL32	HB	1.00	0.000	1.00	0.00
VAL32	HG11	1.00	0.000	1.00	0.00
VAL32	HG21	1.00	0.000	1.00	0.00
VAL32	H	1.00	0.000	1.00	0.00
LEU33	H	0.98	0.000	1.00	0.00

**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	0.00
VAL32	HB	1.00	0.000	1.00	0.00
VAL32	HG11	1.00	0.000	1.00	0.00
VAL32	HG21	1.00	0.000	1.00	0.00
VAL32	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
PRO31	HB2	1.00	0.000	1.00	0.00
PRO31	HB3	1.00	0.000	1.00	0.00
PRO31	HG2	0.89	0.000	1.00	0.00
PRO31	HG3	0.70	0.000	1.00	0.00
VAL32	HA	1.00	0.000	1.00	0.00
VAL32	HB	1.00	0.000	1.00	0.00
VAL32	HG11	1.00	0.000	1.00	0.00
VAL32	HG21	1.00	0.000	1.00	0.00
VAL32	H	1.00	0.000	1.00	0.00
LEU33	H	1.00	0.000	1.00	0.00

**3.32.6 Detailed Probabilities of VAL32HA:**

Overall probability: 0.730

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO31	0.43	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	0.037	0.30	0.00
PRO31	HG2	0.65	0.024	1.00	0.00
VAL32	HA	1.00	0.000	1.00	0.00
VAL32	HB	1.00	0.000	1.00	0.00
VAL32	HG11	1.00	0.000	1.00	0.00
VAL32	HG21	1.00	0.000	1.00	0.00
VAL32	H	1.00	0.000	1.00	0.00
LEU33	HA	1.00	0.399	0.00	0.00
LEU33	H	1.00	0.000	1.00	0.00

**3.32.7 Detailed Probabilities of VAL32HB:**

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
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	0.000	1.00	0.00
VAL32	HB	1.00	0.000	1.00	0.00
VAL32	HG11	1.00	0.000	1.00	0.00
VAL32	HG21	1.00	0.000	1.00	0.00
VAL32	H	1.00	0.000	1.00	0.00
LEU33	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
VAL32	HB	1.00	0.000	1.00	0.00
VAL32	HG11	1.00	0.000	1.00	0.00
VAL32	HG21	1.00	0.000	1.00	0.00
VAL32	H	1.00	0.000	1.00	0.00
LEU33	H	0.98	0.000	1.00	0.00

**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	0.000	1.00	0.00
VAL32	HB	1.00	0.000	1.00	0.00
VAL32	HG11	1.00	0.000	1.00	0.00
VAL32	HG21	1.00	0.000	1.00	0.00
VAL32	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
PRO31	HB2	1.00	0.000	1.00	0.00
PRO31	HB3	1.00	0.000	1.00	0.00
VAL32	HA	1.00	0.000	1.00	0.00
VAL32	HB	1.00	0.000	1.00	0.00
VAL32	HG11	1.00	0.000	1.00	0.00
VAL32	HG21	1.00	0.000	1.00	0.00
VAL32	H	1.00	0.000	1.00	0.00
LEU33	H	1.00	0.000	1.00	0.00

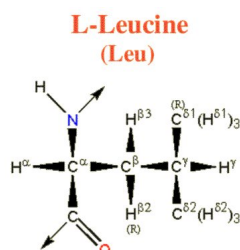
**3.33 LEU(33)**

Figure 23: Image from the BMRB

Residue probability: 0.950

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	0.800	1.000
CB 3.33.2	43.015	42.389	3.750	0.875	1.000
CG 3.33.3	27.248	26.892	3.086	0.878	1.000
CD1 3.33.4	27.157	24.837	3.657	1.000	1.000
CD2 3.33.5	23.739	24.201	3.117	1.000	1.000
N 3.33.6	118.002	121.785	4.943	1.000	1.000
HA 3.33.7	4.635	4.315	0.840	0.800	1.000
HB2 3.33.8	1.648	1.601	0.373	1.000	1.000
HB3 3.33.9	1.521	1.508	0.398	1.000	1.000
HG 3.33.10	1.596	1.510	0.340	1.000	1.000
HD1 3.33.11	0.852	0.739	0.294	1.000	1.000
HD2 3.33.12	0.911	0.727	0.421	1.000	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: 0.800

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL32	0.00	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	0.399	0.00	0.00
LEU33	HA	1.00	0.000	1.00	0.00
LEU33	HB2	1.00	0.000	1.00	0.00
LEU33	HB3	1.00	0.000	1.00	0.00
LEU33	HG	1.00	0.000	1.00	0.00
LEU33	HD11	0.99	0.000	1.00	0.00
LEU33	HD21	0.99	0.000	1.00	0.00
LEU33	H	1.00	0.000	1.00	0.00
GLU34	HA	1.00	0.565	0.00	0.00
GLU34	H	1.00	0.000	1.00	0.00

**3.33.2 Detailed Probabilities of LEU33CB:**

Overall probability: 0.875

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU33	1.00	1.00
GLU34	0.00	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**

### 3.33 LEU(33)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU33	HA	1.00	0.000	1.00	0.00
LEU33	HB2	1.00	0.000	1.00	0.00
LEU33	HB3	1.00	0.000	1.00	0.00
LEU33	HG	1.00	0.000	1.00	0.00
LEU33	HD11	1.00	0.000	1.00	0.00
LEU33	HD21	1.00	0.000	1.00	0.00
LEU33	H	1.00	0.000	1.00	0.00
GLU34	H	1.00	1.431	0.00	0.00

#### 3.33.3 Detailed Probabilities of LEU33CG:

Overall probability: 0.878

Overall confidence: 1.000

##### Inter- and intra-residue probability

Residue	Probability	Confidence
LEU33	1.00	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	0.000	1.00	0.00
LEU33	HB2	1.00	0.000	1.00	0.00
LEU33	HB3	1.00	0.000	1.00	0.00
LEU33	HG	1.00	0.000	1.00	0.00
LEU33	HD11	1.00	0.000	1.00	0.00
LEU33	HD21	1.00	0.000	1.00	0.00
LEU33	H	1.00	0.000	1.00	0.00
GLU34	H	0.98	1.431	0.02	0.00

#### 3.33.4 Detailed Probabilities of LEU33CD1:

Overall probability: 1.000

Overall confidence: 1.000

##### Inter- and intra-residue probability

Residue	Probability	Confidence
LEU33	1.00	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	0.000	1.00	0.00
LEU33	HB2	1.00	0.000	1.00	0.00
LEU33	HB3	1.00	0.000	1.00	0.00
LEU33	HG	1.00	0.000	1.00	0.00
LEU33	HD11	1.00	0.000	1.00	0.00
LEU33	HD21	1.00	0.000	1.00	0.00
LEU33	H	0.86	0.000	1.00	0.00

**3.33.5 Detailed Probabilities of LEU33CD2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU33	1.00	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	0.000	1.00	0.00
LEU33	HB2	1.00	0.000	1.00	0.00
LEU33	HB3	1.00	0.000	1.00	0.00
LEU33	HG	1.00	0.000	1.00	0.00
LEU33	HD11	1.00	0.000	1.00	0.00
LEU33	HD21	1.00	0.000	1.00	0.00
LEU33	H	0.85	0.000	1.00	0.00

**3.33.6 Detailed Probabilities of LEU33N:**

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	0.000	1.00	0.00
VAL32	HB	1.00	0.000	1.00	0.00
VAL32	HG11	0.98	0.000	1.00	0.00
VAL32	H	1.00	0.000	1.00	0.00
VAL32	HG21	0.94	0.000	1.00	0.00
LEU33	HA	1.00	0.000	1.00	0.00
LEU33	HB2	1.00	0.000	1.00	0.00
LEU33	HB3	1.00	0.000	1.00	0.00
LEU33	HG	1.00	0.000	1.00	0.00
LEU33	H	1.00	0.000	1.00	0.00
LEU33	HD11	0.88	0.000	1.00	0.00
LEU33	HD21	0.87	0.000	1.00	0.00
GLU34	H	1.00	0.000	1.00	0.00
GLU34	HA	0.90	0.010	1.00	0.00
GLU34	HB2	0.55	0.008	1.00	0.00

**3.33.7 Detailed Probabilities of LEU33HA:**

Overall probability: 0.800

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL32	0.00	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	0.417	0.00	0.00
LEU33	HA	1.00	0.000	1.00	0.00
LEU33	HB2	1.00	0.000	1.00	0.00
LEU33	HB3	1.00	0.000	1.00	0.00
LEU33	HG	1.00	0.000	1.00	0.00
LEU33	HD11	0.99	0.000	1.00	0.00
LEU33	HD21	0.99	0.000	1.00	0.00
LEU33	H	1.00	0.000	1.00	0.00
GLU34	HA	1.00	0.178	0.00	0.00
GLU34	H	1.00	0.000	1.00	0.00

**3.33.8 Detailed Probabilities of LEU33HB2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU33	1.00	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	0.000	1.00	0.00
LEU33	HB2	1.00	0.000	1.00	0.00
LEU33	HB3	1.00	0.000	1.00	0.00
LEU33	HG	1.00	0.000	1.00	0.00
LEU33	HD11	1.00	0.000	1.00	0.00
LEU33	HD21	1.00	0.000	1.00	0.00
LEU33	H	1.00	0.000	1.00	0.00
GLU34	H	1.00	0.000	1.00	0.00

## 3.33.9 Detailed Probabilities of LEU33HB3:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
LEU33	1.00	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	0.000	1.00	0.00
LEU33	HB2	1.00	0.000	1.00	0.00
LEU33	HB3	1.00	0.000	1.00	0.00
LEU33	HG	1.00	0.000	1.00	0.00
LEU33	HD11	1.00	0.000	1.00	0.00
LEU33	HD21	1.00	0.000	1.00	0.00
LEU33	H	1.00	0.000	1.00	0.00
GLU34	H	1.00	0.000	1.00	0.00

## 3.33.10 Detailed Probabilities of LEU33HG:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
LEU33	1.00	1.00
GLU34	1.00	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	0.000	1.00	0.00
LEU33	HB2	1.00	0.000	1.00	0.00
LEU33	HB3	1.00	0.000	1.00	0.00
LEU33	HG	1.00	0.000	1.00	0.00
LEU33	HD11	1.00	0.000	1.00	0.00
LEU33	HD21	1.00	0.000	1.00	0.00
LEU33	H	1.00	0.000	1.00	0.00
GLU34	H	0.98	0.000	1.00	0.00

**3.33.11 Detailed Probabilities of LEU33HD11:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU33	1.00	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	0.000	1.00	0.00
LEU33	HB2	1.00	0.000	1.00	0.00
LEU33	HB3	1.00	0.000	1.00	0.00
LEU33	HG	1.00	0.000	1.00	0.00
LEU33	HD11	1.00	0.000	1.00	0.00
LEU33	HD21	1.00	0.000	1.00	0.00
LEU33	H	0.86	0.000	1.00	0.00

**3.33.12 Detailed Probabilities of LEU33HD21:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU33	1.00	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	0.000	1.00	0.00
LEU33	HB2	1.00	0.000	1.00	0.00
LEU33	HB3	1.00	0.000	1.00	0.00
LEU33	HG	1.00	0.000	1.00	0.00
LEU33	HD11	1.00	0.000	1.00	0.00
LEU33	HD21	1.00	0.000	1.00	0.00
LEU33	H	0.85	0.000	1.00	0.00

**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	0.000	1.00	0.00
VAL32	HB	1.00	0.000	1.00	0.00
VAL32	HG11	0.98	0.000	1.00	0.00
VAL32	H	1.00	0.000	1.00	0.00
VAL32	HG21	0.94	0.000	1.00	0.00
LEU33	HA	1.00	0.000	1.00	0.00
LEU33	HB2	1.00	0.000	1.00	0.00
LEU33	HB3	1.00	0.000	1.00	0.00
LEU33	HG	1.00	0.000	1.00	0.00
LEU33	H	1.00	0.000	1.00	0.00
LEU33	HD11	0.88	0.000	1.00	0.00
LEU33	HD21	0.87	0.000	1.00	0.00
GLU34	H	1.00	0.000	1.00	0.00

### L-Glutamic Acid (Glu)

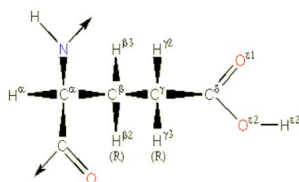


Figure 24: Image from the BMRB

Residue probability confidence: 0.811

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	0.750	0.889
CB 3.34.2	29.929	30.185	4.018	1.000	0.750
CG 3.34.3	36.955	36.085	1.533	1.000	0.750
N 3.34.4	119.011	120.574	4.837	1.000	0.917
HA 3.34.5	4.052	4.245	0.429	0.778	0.889
HB2 3.34.6	2.325	2.021	0.233	1.000	0.750
HB3 3.34.7	2.323	1.994	0.244	1.000	0.750
HG2 3.34.8	2.234	2.258	0.226	1.000	0.750
HG3 3.34.9	2.235	2.233	0.232	1.000	0.750
H 3.34.10	8.997	8.332	0.601	0.771	0.917
HE2	NA	–	–	0.000	0.000

Overall confidence: 0.889

Residue	Probability	Confidence
LEU33	0.00	1.00
GLU34	1.00	1.00
THR35	0.00	0.50

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	0.178	0.00	0.00
GLU34	HA	1.00	0.000	1.00	0.00
GLU34	HB2	1.00	0.000	1.00	0.00
GLU34	HB3	1.00	0.000	1.00	0.00
GLU34	HG2	1.00	0.000	1.00	0.00
GLU34	HG3	1.00	0.000	1.00	0.00
GLU34	H	1.00	0.000	1.00	0.00
THR35	HA	1.00	0.062	0.00	0.00

**3.34.2 Detailed Probabilities of GLU34CB:**

Overall probability: 1.000

Overall confidence: 0.750

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU34	1.00	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	0.000	1.00	0.00
GLU34	HB2	1.00	0.000	1.00	0.00
GLU34	HB3	1.00	0.000	1.00	0.00
GLU34	HG2	1.00	0.000	1.00	0.00
GLU34	HG3	1.00	0.000	1.00	0.00
GLU34	H	1.00	0.000	1.00	0.00

**3.34.3 Detailed Probabilities of GLU34CG:**

Overall probability: 1.000

Overall confidence: 0.750

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU34	1.00	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	0.000	1.00	0.00
GLU34	HB2	1.00	0.000	1.00	0.00
GLU34	HB3	1.00	0.000	1.00	0.00
GLU34	HG2	1.00	0.000	1.00	0.00
GLU34	HG3	1.00	0.000	1.00	0.00
GLU34	H	1.00	0.000	1.00	0.00

**3.34.4 Detailed Probabilities of GLU34N:**

Overall probability: 1.000

Overall confidence: 0.917

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU33	1.00	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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU33	HA	1.00	0.000	1.00	0.00
LEU33	HB2	1.00	0.000	1.00	0.00
LEU33	HB3	1.00	0.000	1.00	0.00
LEU33	HG	0.98	0.000	1.00	0.00
LEU33	H	1.00	0.000	1.00	0.00
LEU33	HD11	0.51	0.000	1.00	0.00
LEU33	HD21	0.58	0.000	1.00	0.00
GLU34	HA	1.00	0.000	1.00	0.00
GLU34	HB2	1.00	0.000	1.00	0.00
GLU34	HB3	1.00	0.000	1.00	0.00
GLU34	HG2	1.00	0.000	1.00	0.00
GLU34	HG3	1.00	0.000	1.00	0.00
GLU34	H	1.00	0.000	1.00	0.00

## 3.34.5 Detailed Probabilities of GLU34HA:

Overall probability: 0.778

Overall confidence: 0.889

## Inter- and intra-residue probability

Residue	Probability	Confidence
LEU33	0.50	1.00
GLU34	1.00	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	0.565	0.00	0.00
LEU33	H	0.90	0.010	1.00	0.00
GLU34	HA	1.00	0.000	1.00	0.00
GLU34	HB2	1.00	0.000	1.00	0.00
GLU34	HB3	1.00	0.000	1.00	0.00
GLU34	HG2	1.00	0.000	1.00	0.00
GLU34	HG3	1.00	0.000	1.00	0.00
GLU34	H	1.00	0.000	1.00	0.00
THR35	HA	1.00	0.343	0.00	0.00

**3.34.6 Detailed Probabilities of GLU34HB2:**

Overall probability: 1.000

Overall confidence: 0.750

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU34	1.00	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	0.000	1.00	0.00
GLU34	HB2	1.00	0.000	1.00	0.00
GLU34	HB3	1.00	0.000	1.00	0.00
GLU34	HG2	1.00	0.000	1.00	0.00
GLU34	HG3	1.00	0.000	1.00	0.00
GLU34	H	1.00	0.000	1.00	0.00

**3.34.7 Detailed Probabilities of GLU34HB3:**

Overall probability: 1.000

Overall confidence: 0.750

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU34	1.00	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	0.000	1.00	0.00
GLU34	HB2	1.00	0.000	1.00	0.00
GLU34	HB3	1.00	0.000	1.00	0.00
GLU34	HG2	1.00	0.000	1.00	0.00
GLU34	HG3	1.00	0.000	1.00	0.00
GLU34	H	1.00	0.000	1.00	0.00

**3.34.8 Detailed Probabilities of GLU34HG2:**

Overall probability: 1.000

Overall confidence: 0.750

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU34	1.00	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	0.000	1.00	0.00
GLU34	HB2	1.00	0.000	1.00	0.00
GLU34	HB3	1.00	0.000	1.00	0.00
GLU34	HG2	1.00	0.000	1.00	0.00
GLU34	HG3	1.00	0.000	1.00	0.00
GLU34	H	1.00	0.000	1.00	0.00

**3.34.9 Detailed Probabilities of GLU34HG3:**

Overall probability: 1.000

Overall confidence: 0.750

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU34	1.00	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	0.000	1.00	0.00
GLU34	HB2	1.00	0.000	1.00	0.00
GLU34	HB3	1.00	0.000	1.00	0.00
GLU34	HG2	1.00	0.000	1.00	0.00
GLU34	HG3	1.00	0.000	1.00	0.00
GLU34	H	1.00	0.000	1.00	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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU33	HA	1.00	0.000	1.00	0.00
LEU33	HB2	1.00	1.431	0.00	0.00
LEU33	HB3	1.00	1.431	0.00	0.00
LEU33	HG	0.98	1.431	0.02	0.00
LEU33	H	1.00	0.000	1.00	0.00
LEU33	HD11	0.51	0.004	1.00	0.00
LEU33	HD21	0.58	0.000	1.00	0.00
GLU34	HA	1.00	0.000	1.00	0.00
GLU34	HB2	1.00	0.000	1.00	0.00
GLU34	HB3	1.00	0.000	1.00	0.00
GLU34	HG2	1.00	0.000	1.00	0.00
GLU34	HG3	1.00	0.000	1.00	0.00
GLU34	H	1.00	0.000	1.00	0.00

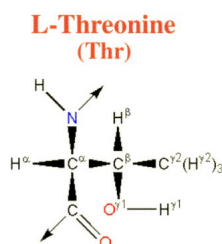


Figure 25: Image from the BMRB

Residue probability: 0.903  
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	0.750	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	1.000	0.667
N	NA	—	—	0.000	0.000
HA 3.35.4	4.395	4.461	0.626	0.667	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: 0.750  
Overall confidence: 0.750

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU34	0.67	1.00
THR35	1.00	0.60
ARG36	0.50	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	0.343	0.00	0.00
GLU34	HB2	0.64	0.016	1.00	0.00
GLU34	HB3	0.81	0.014	1.00	0.00
THR35	HA	1.00	0.000	1.00	0.00
THR35	HB	1.00	0.000	1.00	0.00
THR35	HG21	1.00	0.000	1.00	0.00
ARG36	HA	1.00	0.236	0.00	0.00
ARG36	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
THR35	HB	1.00	0.000	1.00	0.00
THR35	HG21	1.00	0.000	1.00	0.00
ARG36	H	1.00	0.000	1.00	0.00

**3.35.3 Detailed Probabilities of THR35CG2:**

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	0.000	1.00	0.00
THR35	HB	1.00	0.000	1.00	0.00
THR35	HG21	1.00	0.000	1.00	0.00
ARG36	H	0.95	0.000	1.00	0.00

**3.35.4 Detailed Probabilities of THR35HA:**

Overall probability: 0.667

Overall confidence: 0.750

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU34	0.00	1.00
THR35	1.00	0.60
ARG36	0.50	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	0.062	0.00	0.00
THR35	HA	1.00	0.000	1.00	0.00
THR35	HB	1.00	0.000	1.00	0.00
THR35	HG21	1.00	0.000	1.00	0.00
ARG36	HA	1.00	0.340	0.00	0.00
ARG36	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
THR35	HB	1.00	0.000	1.00	0.00
THR35	HG21	1.00	0.000	1.00	0.00
ARG36	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
THR35	HB	1.00	0.000	1.00	0.00
THR35	HG21	1.00	0.000	1.00	0.00
ARG36	H	0.95	0.000	1.00	0.00

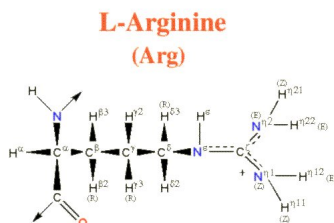


Figure 26: Image from the BMRB

Residue probability: 0.947  
 Residue probability confidence: 0.837

#### 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	0.702	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	0.800
CD 3.36.4	43.472	43.189	1.415	1.000	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	0.800	1.000
HB2 3.36.7	2.027	1.793	0.292	1.000	0.889
HB3 3.36.8	1.898	1.757	0.307	1.000	0.889
HG2 3.36.9	1.622	1.559	0.294	1.000	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	0.861	0.667
H 3.36.12	7.318	8.248	0.623	1.000	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: 0.702  
 Overall confidence: 1.000

#### Inter- and intra-residue probability

Residue	Probability	Confidence
THR35	0.00	1.00
ARG36	0.86	1.00
THR37	0.50	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	0.340	0.00	0.00
ARG36	HA	1.00	0.000	1.00	0.00
ARG36	HB2	1.00	0.000	1.00	0.00
ARG36	HB3	1.00	0.000	1.00	0.00
ARG36	HG2	1.00	0.000	1.00	0.00
ARG36	HG3	1.00	0.000	1.00	0.00
ARG36	HD2	0.98	1.154	0.02	0.00
ARG36	H	1.00	0.000	1.00	0.00
THR37	HA	1.00	0.171	0.00	0.00
THR37	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ARG36	HB2	1.00	0.000	1.00	0.00
ARG36	HB3	1.00	0.000	1.00	0.00
ARG36	HG2	1.00	0.000	1.00	0.00
ARG36	HG3	1.00	0.000	1.00	0.00
ARG36	HD2	1.00	0.000	1.00	0.00
ARG36	H	1.00	0.000	1.00	0.00
THR37	H	1.00	0.000	1.00	0.00
THR37	HA	0.66	0.025	1.00	0.00

## 3.36.3 Detailed Probabilities of ARG36CG:

Overall probability: 1.000

Overall confidence: 0.800

## Inter- and intra-residue probability

Residue	Probability	Confidence
ARG36	1.00	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	0.000	1.00	0.00
ARG36	HB2	1.00	0.000	1.00	0.00
ARG36	HB3	1.00	0.000	1.00	0.00
ARG36	HG2	1.00	0.000	1.00	0.00
ARG36	HG3	1.00	0.000	1.00	0.00
ARG36	HD2	1.00	0.000	1.00	0.00
ARG36	H	1.00	0.000	1.00	0.00
THR37	H	0.97	0.000	1.00	0.00

## 3.36.4 Detailed Probabilities of ARG36CD:

Overall probability: 1.000

Overall confidence: 0.667

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ARG36	1.00	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	0.000	1.00	0.00
ARG36	HB2	1.00	0.000	1.00	0.00
ARG36	HB3	1.00	0.000	1.00	0.00
ARG36	HG2	1.00	0.000	1.00	0.00
ARG36	HG3	1.00	0.000	1.00	0.00
ARG36	HD2	1.00	0.000	1.00	0.00
ARG36	H	0.86	0.000	1.00	0.00

**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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR35	HA	1.00	0.000	1.00	0.00
THR35	HB	1.00	0.000	1.00	0.00
THR35	HG21	0.96	0.000	1.00	0.00
ARG36	HA	1.00	0.000	1.00	0.00
ARG36	HB2	1.00	0.000	1.00	0.00
ARG36	HB3	1.00	0.000	1.00	0.00
ARG36	HG2	1.00	0.000	1.00	0.00
ARG36	HG3	1.00	0.000	1.00	0.00
ARG36	H	1.00	0.000	1.00	0.00
ARG36	HD2	0.87	0.000	1.00	0.00
THR37	H	1.00	0.000	1.00	0.00

**3.36.6 Detailed Probabilities of ARG36HA:**

Overall probability: 0.800

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR35	0.00	1.00
ARG36	1.00	1.00
THR37	0.50	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	0.236	0.00	0.00
ARG36	HA	1.00	0.000	1.00	0.00
ARG36	HB2	1.00	0.000	1.00	0.00
ARG36	HB3	1.00	0.000	1.00	0.00
ARG36	HG2	1.00	0.000	1.00	0.00
ARG36	HG3	1.00	0.000	1.00	0.00
ARG36	HD2	0.98	0.000	1.00	0.00
ARG36	H	1.00	0.000	1.00	0.00
THR37	HA	1.00	0.171	0.00	0.00
THR37	H	1.00	0.000	1.00	0.00

**3.36.7 Detailed Probabilities of ARG36HB2:**

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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG36	HA	1.00	0.000	1.00	0.00
ARG36	HB2	1.00	0.000	1.00	0.00
ARG36	HB3	1.00	0.000	1.00	0.00
ARG36	HG2	1.00	0.000	1.00	0.00
ARG36	HG3	1.00	0.000	1.00	0.00
ARG36	HD2	1.00	0.000	1.00	0.00
ARG36	H	1.00	0.000	1.00	0.00
THR37	H	1.00	0.000	1.00	0.00

**3.36.8 Detailed Probabilities of ARG36HB3:**

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
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	0.000	1.00	0.00
ARG36	HB2	1.00	0.000	1.00	0.00
ARG36	HB3	1.00	0.000	1.00	0.00
ARG36	HG2	1.00	0.000	1.00	0.00
ARG36	HG3	1.00	0.000	1.00	0.00
ARG36	HD2	1.00	0.000	1.00	0.00
ARG36	H	1.00	0.000	1.00	0.00
THR37	H	1.00	0.000	1.00	0.00

**3.36.9 Detailed Probabilities of ARG36HG2:**

Overall probability: 1.000

Overall confidence: 0.800

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ARG36	1.00	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	0.000	1.00	0.00
ARG36	HB2	1.00	0.000	1.00	0.00
ARG36	HB3	1.00	0.000	1.00	0.00
ARG36	HG2	1.00	0.000	1.00	0.00
ARG36	HG3	1.00	0.000	1.00	0.00
ARG36	HD2	1.00	0.000	1.00	0.00
ARG36	H	1.00	0.000	1.00	0.00
THR37	H	0.97	0.000	1.00	0.00

**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	0.000	1.00	0.00
ARG36	HB2	1.00	0.000	1.00	0.00
ARG36	HB3	1.00	0.000	1.00	0.00
ARG36	HG2	1.00	0.000	1.00	0.00
ARG36	HG3	1.00	0.000	1.00	0.00
ARG36	HD2	1.00	0.000	1.00	0.00
ARG36	H	1.00	0.000	1.00	0.00

**3.36.11 Detailed Probabilities of ARG36HD2:**

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**

## 3.36 ARG(36)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG36	HA	0.97	1.154	0.03	0.00
ARG36	HB2	1.00	0.000	1.00	0.00
ARG36	HB3	1.00	0.000	1.00	0.00
ARG36	HG2	1.00	0.000	1.00	0.00
ARG36	HG3	1.00	0.000	1.00	0.00
ARG36	HD2	1.00	0.000	1.00	0.00
ARG36	H	0.86	0.000	1.00	0.00

## 3.36.12 Detailed Probabilities of ARG36H:

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

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR35	HA	1.00	0.000	1.00	0.00
THR35	HB	1.00	0.000	1.00	0.00
THR35	HG21	0.96	0.000	1.00	0.00
ARG36	HA	1.00	0.000	1.00	0.00
ARG36	HB2	1.00	0.000	1.00	0.00
ARG36	HB3	1.00	0.000	1.00	0.00
ARG36	HG2	1.00	0.000	1.00	0.00
ARG36	HG3	1.00	0.000	1.00	0.00
ARG36	H	1.00	0.000	1.00	0.00
ARG36	HD2	0.87	0.000	1.00	0.00
THR37	H	1.00	0.000	1.00	0.00

**3.37 THR(37)**

Figure 27: Image from the BMRB

Residue probability: 0.937

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	0.714	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	0.778	0.875
HB 3.37.6	4.260	4.172	0.855	1.000	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	1.000	0.909
HG1	NA	—	—	0.000	0.000

**3.37.1 Detailed Probabilities of THR37CA:**

Overall probability: 0.714

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ARG36	0.00	1.00
THR37	1.00	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	0.171	0.00	0.00
THR37	HA	1.00	0.000	1.00	0.00
THR37	HB	1.00	0.000	1.00	0.00
THR37	HG21	1.00	0.000	1.00	0.00
THR37	H	1.00	0.000	1.00	0.00
MET38	HA	1.00	0.075	0.00	0.00
MET38	H	1.00	0.000	1.00	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	0.000	1.00	0.00
THR37	HB	1.00	0.000	1.00	0.00
THR37	HG21	1.00	0.000	1.00	0.00
THR37	H	1.00	0.000	1.00	0.00
MET38	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
THR37	HB	1.00	0.000	1.00	0.00
THR37	HG21	1.00	0.000	1.00	0.00
THR37	H	1.00	0.000	1.00	0.00
MET38	H	0.97	0.000	1.00	0.00

**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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG36	HA	1.00	0.000	1.00	0.00
ARG36	HB2	1.00	0.000	1.00	0.00
ARG36	HB3	1.00	0.000	1.00	0.00
ARG36	HG2	0.97	0.000	1.00	0.00
ARG36	H	1.00	0.000	1.00	0.00
ARG36	HG3	0.94	0.000	1.00	0.00
ARG36	HD2	0.57	0.000	1.00	0.00
THR37	HA	1.00	0.000	1.00	0.00
THR37	HB	1.00	0.000	1.00	0.00
THR37	HG21	1.00	0.000	1.00	0.00
THR37	H	1.00	0.000	1.00	0.00
MET38	H	1.00	0.000	1.00	0.00
MET38	HB2	0.55	0.011	1.00	0.00

## 3.37.5 Detailed Probabilities of THR37HA:

Overall probability: 0.778

Overall confidence: 0.875

## Inter- and intra-residue probability

Residue	Probability	Confidence
ARG36	0.67	1.00
THR37	1.00	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	0.171	0.00	0.00
ARG36	HB2	0.66	0.025	1.00	0.00
ARG36	HB3	0.82	0.018	1.00	0.00
THR37	HA	1.00	0.000	1.00	0.00
THR37	HB	1.00	0.000	1.00	0.00
THR37	HG21	1.00	0.000	1.00	0.00
THR37	H	1.00	0.000	1.00	0.00
MET38	HA	1.00	0.721	0.00	0.00
MET38	H	1.00	0.000	1.00	0.00

**3.37.6 Detailed Probabilities of THR37HB:**

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	0.000	1.00	0.00
THR37	HB	1.00	0.000	1.00	0.00
THR37	HG21	1.00	0.000	1.00	0.00
THR37	H	1.00	0.000	1.00	0.00
MET38	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
THR37	HB	1.00	0.000	1.00	0.00
THR37	HG21	1.00	0.000	1.00	0.00
THR37	H	1.00	0.000	1.00	0.00
MET38	H	0.97	0.000	1.00	0.00

**3.37.8 Detailed Probabilities of THR37H:**

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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG36	HA	1.00	0.000	1.00	0.00
ARG36	HB2	1.00	0.000	1.00	0.00
ARG36	HB3	1.00	0.000	1.00	0.00
ARG36	HG2	0.97	0.000	1.00	0.00
ARG36	H	1.00	0.000	1.00	0.00
ARG36	HG3	0.94	0.000	1.00	0.00
ARG36	HD2	0.57	0.000	1.00	0.00
THR37	HA	1.00	0.000	1.00	0.00
THR37	HB	1.00	0.000	1.00	0.00
THR37	HG21	1.00	0.000	1.00	0.00
THR37	H	1.00	0.000	1.00	0.00
MET38	H	1.00	0.000	1.00	0.00

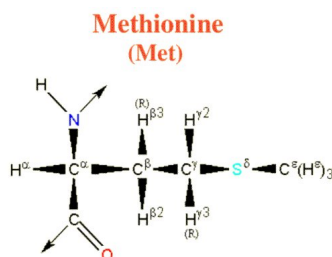
**3.38 MET(38)**

Figure 28: Image from the BMRB

Residue probability: 0.970

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	0.818	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	1.000	1.000
N 3.38.5	118.861	120.023	5.158	1.000	0.917
HA 3.38.6	4.185	4.409	0.504	0.818	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	1.000	1.000
HG2 3.38.9	2.108	2.410	0.360	1.000	1.000
HG3 3.38.10	1.750	2.378	0.386	1.000	1.000
HE 3.38.11	2.005	1.877	0.381	1.000	1.000
H 3.38.12	8.376	8.269	0.585	1.000	0.917

**3.38.1 Detailed Probabilities of MET38CA:**

Overall probability: 0.818

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR37	0.00	1.00
MET38	1.00	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	0.721	0.00	0.00
MET38	HA	1.00	0.000	1.00	0.00
MET38	HB2	1.00	0.000	1.00	0.00
MET38	HB3	1.00	0.000	1.00	0.00
MET38	HG2	1.00	0.000	1.00	0.00
MET38	HG3	1.00	0.000	1.00	0.00
MET38	H	1.00	0.000	1.00	0.00
MET38	HE1	0.69	0.000	1.00	0.00
ASP39	HA	1.00	0.857	0.00	0.00
ASP39	H	1.00	0.000	1.00	0.00
ASP39	HB2	0.54	0.011	1.00	0.00

**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	0.000	1.00	0.00
MET38	HB2	1.00	0.000	1.00	0.00
MET38	HB3	1.00	0.000	1.00	0.00
MET38	HG2	1.00	0.000	1.00	0.00
MET38	HG3	1.00	0.000	1.00	0.00
MET38	HE1	0.96	0.000	1.00	0.00
MET38	H	1.00	0.000	1.00	0.00
ASP39	H	1.00	0.000	1.00	0.00

## 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
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	0.000	1.00	0.00
MET38	HB2	1.00	0.000	1.00	0.00
MET38	HB3	1.00	0.000	1.00	0.00
MET38	HG2	1.00	0.000	1.00	0.00
MET38	HG3	1.00	0.000	1.00	0.00
MET38	HE1	1.00	0.000	1.00	0.00
MET38	H	1.00	0.000	1.00	0.00
ASP39	H	0.97	0.000	1.00	0.00

## 3.38.4 Detailed Probabilities of MET38CE:

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
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	0.000	1.00	0.00
MET38	HB3	0.97	0.000	1.00	0.00
MET38	HG2	1.00	0.000	1.00	0.00
MET38	HG3	1.00	0.000	1.00	0.00
MET38	HE1	1.00	0.000	1.00	0.00
MET38	HA	0.67	0.000	1.00	0.00

**3.38.5 Detailed Probabilities of MET38N:**

Overall probability: 1.000

Overall confidence: 0.917

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR37	1.00	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**

## 3.38 MET(38)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR37	HA	1.00	0.000	1.00	0.00
THR37	HB	1.00	0.000	1.00	0.00
THR37	HG21	0.97	0.000	1.00	0.00
THR37	H	1.00	0.000	1.00	0.00
MET38	HA	1.00	0.000	1.00	0.00
MET38	HB2	1.00	0.000	1.00	0.00
MET38	HB3	1.00	0.000	1.00	0.00
MET38	HG2	1.00	0.000	1.00	0.00
MET38	HG3	1.00	0.000	1.00	0.00
MET38	H	1.00	0.000	1.00	0.00
ASP39	H	1.00	0.024	1.00	0.00

## 3.38.6 Detailed Probabilities of MET38HA:

Overall probability: 0.818

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
THR37	0.00	1.00
MET38	1.00	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	0.075	0.00	0.00
MET38	HA	1.00	0.000	1.00	0.00
MET38	HB2	1.00	0.000	1.00	0.00
MET38	HB3	1.00	0.000	1.00	0.00
MET38	HG2	1.00	0.000	1.00	0.00
MET38	HG3	1.00	0.000	1.00	0.00
MET38	H	1.00	0.000	1.00	0.00
MET38	HE1	0.69	0.000	1.00	0.00
ASP39	HA	1.00	0.857	0.00	0.00
ASP39	H	1.00	0.000	1.00	0.00
ASP39	HB2	0.54	0.001	1.00	0.00

**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	0.000	1.00	0.00
MET38	HB2	1.00	0.000	1.00	0.00
MET38	HB3	1.00	0.000	1.00	0.00
MET38	HG2	1.00	0.000	1.00	0.00
MET38	HG3	1.00	0.000	1.00	0.00
MET38	HE1	0.96	0.000	1.00	0.00
MET38	H	1.00	0.000	1.00	0.00
ASP39	H	1.00	0.000	1.00	0.00

**3.38.8 Detailed Probabilities of MET38HB3:**

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
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	0.000	1.00	0.00
MET38	HB2	1.00	0.000	1.00	0.00
MET38	HB3	1.00	0.000	1.00	0.00
MET38	HG2	1.00	0.000	1.00	0.00
MET38	HG3	1.00	0.000	1.00	0.00
MET38	HE1	0.97	0.000	1.00	0.00
MET38	H	1.00	0.000	1.00	0.00
ASP39	H	1.00	0.000	1.00	0.00

**3.38.9 Detailed Probabilities of MET38HG2:**

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
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	0.000	1.00	0.00
MET38	HB2	1.00	0.000	1.00	0.00
MET38	HB3	1.00	0.000	1.00	0.00
MET38	HG2	1.00	0.000	1.00	0.00
MET38	HG3	1.00	0.000	1.00	0.00
MET38	HE1	1.00	0.000	1.00	0.00
MET38	H	1.00	0.000	1.00	0.00
ASP39	H	0.97	0.000	1.00	0.00

**3.38.10 Detailed Probabilities of MET38HG3:**

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	0.000	1.00	0.00
MET38	HB2	1.00	0.000	1.00	0.00
MET38	HB3	1.00	0.000	1.00	0.00
MET38	HG2	1.00	0.000	1.00	0.00
MET38	HG3	1.00	0.000	1.00	0.00
MET38	HE1	1.00	0.000	1.00	0.00
MET38	H	1.00	0.000	1.00	0.00

**3.38.11 Detailed Probabilities of MET38HE1:**

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
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	0.000	1.00	0.00
MET38	HB3	0.97	0.000	1.00	0.00
MET38	HG2	1.00	0.000	1.00	0.00
MET38	HG3	1.00	0.000	1.00	0.00
MET38	HE1	1.00	0.000	1.00	0.00
MET38	HA	0.67	0.000	1.00	0.00

**3.38.12 Detailed Probabilities of MET38H:**

Overall probability: 1.000

Overall confidence: 0.917

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR37	1.00	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	0.000	1.00	0.00
THR37	HB	1.00	0.000	1.00	0.00
THR37	HG21	0.97	0.000	1.00	0.00
THR37	H	1.00	0.000	1.00	0.00
MET38	HA	1.00	0.000	1.00	0.00
MET38	HB2	1.00	0.000	1.00	0.00
MET38	HB3	1.00	0.000	1.00	0.00
MET38	HG2	1.00	0.000	1.00	0.00
MET38	HG3	1.00	0.000	1.00	0.00
MET38	H	1.00	0.000	1.00	0.00
ASP39	H	1.00	0.024	1.00	0.00
ASP39	HA	0.85	0.024	1.00	0.00
ASP39	HB2	0.56	0.024	1.00	0.00

**3.39 ASP(39)**

Figure 29: Image from the BMRB

Residue probability: 0.923

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	0.750	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	0.714	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: 0.750

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
MET38	0.50	1.00
ASP39	1.00	0.80
PHE40	0.50	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	0.857	0.00	0.00
MET38	H	0.85	0.024	1.00	0.00
ASP39	HA	1.00	0.000	1.00	0.00
ASP39	HB2	1.00	0.000	1.00	0.00
ASP39	HB3	1.00	0.000	1.00	0.00
ASP39	H	1.00	0.000	1.00	0.00
PHE40	HA	1.00	0.129	0.00	0.00
PHE40	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ASP39	HB2	1.00	0.000	1.00	0.00
ASP39	HB3	1.00	0.000	1.00	0.00
ASP39	H	1.00	0.000	1.00	0.00
PHE40	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
MET38	HB2	1.00	0.000	1.00	0.00
MET38	HB3	1.00	0.000	1.00	0.00
MET38	HG2	0.97	0.000	1.00	0.00
MET38	H	1.00	0.024	1.00	0.00
MET38	HG3	0.95	0.000	1.00	0.00
ASP39	HA	1.00	0.000	1.00	0.00
ASP39	HB2	1.00	0.000	1.00	0.00
ASP39	HB3	1.00	0.000	1.00	0.00
ASP39	H	1.00	0.000	1.00	0.00
PHE40	H	1.00	0.000	1.00	0.00

**3.39.4 Detailed Probabilities of ASP39HA:**

Overall probability: 0.714

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
MET38	0.00	1.00
ASP39	1.00	0.80
PHE40	0.50	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	0.857	0.00	0.00
ASP39	HA	1.00	0.000	1.00	0.00
ASP39	HB2	1.00	0.000	1.00	0.00
ASP39	HB3	1.00	0.000	1.00	0.00
ASP39	H	1.00	0.000	1.00	0.00
PHE40	HA	1.00	0.129	0.00	0.00
PHE40	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ASP39	HB2	1.00	0.000	1.00	0.00
ASP39	HB3	1.00	0.000	1.00	0.00
ASP39	H	1.00	0.000	1.00	0.00
PHE40	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ASP39	HB2	1.00	0.000	1.00	0.00
ASP39	HB3	1.00	0.000	1.00	0.00
ASP39	H	1.00	0.000	1.00	0.00
PHE40	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
MET38	HB2	1.00	0.000	1.00	0.00
MET38	HB3	1.00	0.000	1.00	0.00
MET38	HG2	0.97	0.000	1.00	0.00
MET38	H	1.00	0.024	1.00	0.00
MET38	HG3	0.95	0.000	1.00	0.00
ASP39	HA	1.00	0.000	1.00	0.00
ASP39	HB2	1.00	0.000	1.00	0.00
ASP39	HB3	1.00	0.000	1.00	0.00
ASP39	H	1.00	0.000	1.00	0.00
PHE40	H	1.00	0.000	1.00	0.00

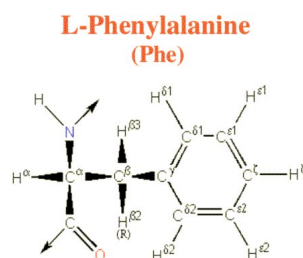
**3.40 PHE(40)**

Figure 30: Image from the BMRB

Residue probability: 0.889

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	0.600	1.000
CB 3.40.2	38.650	40.078	3.616	0.803	1.000
CD1 3.40.3	131.700	131.234	9.579	1.000	1.000
CD2 3.40.4	131.792	131.352	9.581	1.000	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	0.715	1.000
CZ 3.40.7	128.949	129.042	3.448	1.000	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	0.800	1.000
HB2 3.40.10	3.518	2.980	0.399	0.672	1.000
HB3 3.40.11	2.670	2.916	0.434	0.670	1.000
HD1 3.40.12	6.671	7.037	0.347	1.000	1.000
HD2 3.40.13	6.671	7.022	0.417	1.000	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	0.857	1.000
HZ 3.40.16	6.750	6.984	1.598	1.000	1.000
H 3.40.17	8.836	8.375	0.710	1.000	1.000

**3.40.1 Detailed Probabilities of PHE40CA:**

Overall probability: 0.600

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASP39	0.00	1.00
PHE40	1.00	1.00
PRO41	0.00	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	0.129	0.00	0.00
PHE40	HA	1.00	0.000	1.00	0.00
PHE40	HB2	1.00	0.000	1.00	0.00
PHE40	HB3	1.00	0.000	1.00	0.00
PHE40	HD1	1.00	0.000	1.00	0.00
PHE40	HD2	1.00	0.000	1.00	0.00
PHE40	H	1.00	0.000	1.00	0.00
PRO41	HA	1.00	0.293	0.00	0.00
PRO41	HD2	1.00	0.149	0.00	0.00
PRO41	HD3	1.00	0.083	0.00	0.00

**3.40.2 Detailed Probabilities of PHE40CB:**

Overall probability: 0.803

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE40	1.00	1.00
PRO41	0.01	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**

## 3.40 PHE(40)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE40	HA	1.00	0.000	1.00	0.00
PHE40	HB2	1.00	0.000	1.00	0.00
PHE40	HB3	1.00	0.000	1.00	0.00
PHE40	HD1	1.00	0.000	1.00	0.00
PHE40	HD2	1.00	0.000	1.00	0.00
PHE40	HE2	1.00	0.000	1.00	0.00
PHE40	H	1.00	0.000	1.00	0.00
PHE40	HE1	0.89	0.000	1.00	0.00
PRO41	HD2	0.98	0.149	0.02	0.00
PRO41	HD3	0.99	0.083	0.01	0.00

## 3.40.3 Detailed Probabilities of PHE40CD1:

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
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	0.000	1.00	0.00
PHE40	HB2	1.00	0.000	1.00	0.00
PHE40	HB3	1.00	0.000	1.00	0.00
PHE40	HD1	1.00	0.000	1.00	0.00
PHE40	HD2	1.00	0.000	1.00	0.00
PHE40	HE1	1.00	0.000	1.00	0.00
PHE40	HE2	1.00	0.000	1.00	0.00
PHE40	HZ	1.00	0.000	1.00	0.00
PHE40	H	1.00	0.000	1.00	0.00

## 3.40.4 Detailed Probabilities of PHE40CD2:

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
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	0.000	1.00	0.00
PHE40	HB2	1.00	0.000	1.00	0.00
PHE40	HB3	1.00	0.000	1.00	0.00
PHE40	HD1	1.00	0.000	1.00	0.00
PHE40	HD2	1.00	0.000	1.00	0.00
PHE40	HE1	1.00	0.000	1.00	0.00
PHE40	HE2	1.00	0.000	1.00	0.00
PHE40	HZ	1.00	0.000	1.00	0.00
PHE40	H	0.99	0.000	1.00	0.00

**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	0.00
PHE40	HD2	1.00	0.000	1.00	0.00
PHE40	HE1	1.00	0.000	1.00	0.00
PHE40	HE2	1.00	0.000	1.00	0.00
PHE40	HZ	1.00	0.000	1.00	0.00

**3.40.6 Detailed Probabilities of PHE40CE2:**

Overall probability: 0.715

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE40	0.71	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	0.280	0.00	0.00
PHE40	HB3	1.00	0.568	0.00	0.00
PHE40	HD1	1.00	0.000	1.00	0.00
PHE40	HD2	1.00	0.000	1.00	0.00
PHE40	HE1	1.00	0.000	1.00	0.00
PHE40	HE2	1.00	0.000	1.00	0.00
PHE40	HZ	1.00	0.000	1.00	0.00

**3.40.7 Detailed Probabilities of PHE40CZ:**

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
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	0.000	1.00	0.00
PHE40	HD2	1.00	0.000	1.00	0.00
PHE40	HE1	1.00	0.000	1.00	0.00
PHE40	HE2	1.00	0.000	1.00	0.00
PHE40	HZ	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ASP39	HB2	1.00	0.000	1.00	0.00
ASP39	HB3	1.00	0.000	1.00	0.00
ASP39	H	1.00	0.000	1.00	0.00
PHE40	HA	1.00	0.000	1.00	0.00
PHE40	HB2	1.00	0.000	1.00	0.00
PHE40	HB3	1.00	0.000	1.00	0.00
PHE40	HD1	1.00	0.000	1.00	0.00
PHE40	HD2	0.99	0.000	1.00	0.00
PHE40	H	1.00	0.000	1.00	0.00
PRO41	HD2	0.98	0.023	1.00	0.00
PRO41	HD3	0.97	0.005	1.00	0.00

**3.40.9 Detailed Probabilities of PHE40HA:**

Overall probability: 0.800

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASP39	0.00	1.00
PHE40	1.00	1.00
PRO41	0.67	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	0.129	0.00	0.00
PHE40	HA	1.00	0.000	1.00	0.00
PHE40	HB2	1.00	0.000	1.00	0.00
PHE40	HB3	1.00	0.000	1.00	0.00
PHE40	HD1	1.00	0.000	1.00	0.00
PHE40	HD2	1.00	0.000	1.00	0.00
PHE40	H	1.00	0.000	1.00	0.00
PRO41	HA	1.00	0.059	0.00	0.00
PRO41	HD2	1.00	0.016	1.00	0.00
PRO41	HD3	1.00	0.012	1.00	0.00

**3.40.10 Detailed Probabilities of PHE40HB2:**

Overall probability: 0.672

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE40	0.86	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**

## 3.40 PHE(40)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE40	HA	1.00	0.000	1.00	0.00
PHE40	HB2	1.00	0.000	1.00	0.00
PHE40	HB3	1.00	0.000	1.00	0.00
PHE40	HD1	1.00	0.000	1.00	0.00
PHE40	HD2	1.00	0.000	1.00	0.00
PHE40	HE2	1.00	0.280	0.00	0.00
PHE40	H	1.00	0.000	1.00	0.00
PRO41	HD2	0.97	0.069	0.03	0.00
PRO41	HD3	0.98	0.069	0.02	0.00

## 3.40.11 Detailed Probabilities of PHE40HB3:

Overall probability: 0.670

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
PHE40	0.86	1.00
PRO41	0.01	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	0.000	1.00	0.00
PHE40	HB2	1.00	0.000	1.00	0.00
PHE40	HB3	1.00	0.000	1.00	0.00
PHE40	HD1	1.00	0.000	1.00	0.00
PHE40	HD2	1.00	0.000	1.00	0.00
PHE40	HE2	1.00	0.568	0.00	0.00
PHE40	H	1.00	0.000	1.00	0.00
PRO41	HD2	0.98	0.098	0.02	0.00
PRO41	HD3	0.99	0.098	0.01	0.00

## 3.40.12 Detailed Probabilities of PHE40HD1:

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
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	0.000	1.00	0.00
PHE40	HB2	1.00	0.000	1.00	0.00
PHE40	HB3	1.00	0.000	1.00	0.00
PHE40	HD1	1.00	0.000	1.00	0.00
PHE40	HD2	1.00	0.000	1.00	0.00
PHE40	HE1	1.00	0.000	1.00	0.00
PHE40	HE2	1.00	0.000	1.00	0.00
PHE40	HZ	1.00	0.000	1.00	0.00
PHE40	H	1.00	0.000	1.00	0.00

**3.40.13 Detailed Probabilities of PHE40HD2:**

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
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	0.000	1.00	0.00
PHE40	HB2	1.00	0.000	1.00	0.00
PHE40	HB3	1.00	0.000	1.00	0.00
PHE40	HD1	1.00	0.000	1.00	0.00
PHE40	HD2	1.00	0.000	1.00	0.00
PHE40	HE1	1.00	0.000	1.00	0.00
PHE40	HE2	1.00	0.000	1.00	0.00
PHE40	HZ	1.00	0.000	1.00	0.00
PHE40	H	0.99	0.000	1.00	0.00

**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	0.000	1.00	0.00
PHE40	HD2	1.00	0.000	1.00	0.00
PHE40	HE1	1.00	0.000	1.00	0.00
PHE40	HE2	1.00	0.000	1.00	0.00
PHE40	HZ	1.00	0.000	1.00	0.00
PHE40	HB3	0.89	0.000	1.00	0.00

**3.40.15 Detailed Probabilities of PHE40HE2:**

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	0.499	0.00	0.00
PHE40	HB3	1.00	0.000	1.00	0.00
PHE40	HD1	1.00	0.000	1.00	0.00
PHE40	HD2	1.00	0.000	1.00	0.00
PHE40	HE1	1.00	0.000	1.00	0.00
PHE40	HE2	1.00	0.000	1.00	0.00
PHE40	HZ	1.00	0.000	1.00	0.00

**3.40.16 Detailed Probabilities of PHE40HZ:**

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
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	0.000	1.00	0.00
PHE40	HD2	1.00	0.000	1.00	0.00
PHE40	HE1	1.00	0.000	1.00	0.00
PHE40	HE2	1.00	0.000	1.00	0.00
PHE40	HZ	1.00	0.000	1.00	0.00

**3.40.17 Detailed Probabilities of PHE40H:**

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	0.000	1.00	0.00
ASP39	HB2	1.00	0.000	1.00	0.00
ASP39	HB3	1.00	0.000	1.00	0.00
ASP39	H	1.00	0.000	1.00	0.00
PHE40	HA	1.00	0.000	1.00	0.00
PHE40	HB2	1.00	0.000	1.00	0.00
PHE40	HB3	1.00	0.000	1.00	0.00
PHE40	HD1	1.00	0.000	1.00	0.00
PHE40	HD2	0.99	0.000	1.00	0.00
PHE40	H	1.00	0.000	1.00	0.00
PRO41	HD2	0.98	0.002	1.00	0.00
PRO41	HD3	0.97	0.002	1.00	0.00

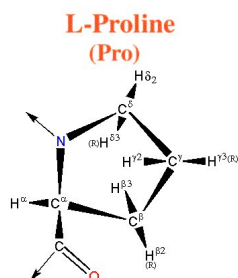


Figure 31: Image from the BMRB

Residue probability: 0.837  
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	15.301	0.667	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	1.000	1.000
CD 3.41.4	50.490	49.797	3.175	0.837	1.000
N	NA	—	—	0.000	0.000
HA 3.41.5	4.620	4.332	0.427	0.778	1.000
HB2 3.41.6	2.486	2.099	0.501	0.877	1.000
HB3 3.41.7	2.114	2.052	0.596	1.000	1.000
HG 3.41.8	2.076	1.927	0.364	1.000	1.000
HD2 3.41.9	3.667	3.640	0.682	0.605	1.000
HD3 3.41.10	3.435	3.558	0.522	0.603	1.000

**3.41.1 Detailed Probabilities of PRO41CA:**

Overall probability: 0.667  
Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE40	0.00	1.00
PRO41	0.67	1.00
THR42	1.00	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	0.059	0.00	0.00
PRO41	HA	1.00	0.000	1.00	0.00
PRO41	HB2	1.00	0.000	1.00	0.00
PRO41	HB3	1.00	0.000	1.00	0.00
PRO41	HG2	1.00	0.000	1.00	0.00
PRO41	HD2	1.00	0.268	0.00	0.00
PRO41	HD3	1.00	0.500	0.00	0.00
THR42	HA	1.00	0.008	1.00	0.00
THR42	H	1.00	0.000	1.00	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	0.000	1.00	0.00
PRO41	HB2	1.00	0.000	1.00	0.00
PRO41	HB3	1.00	0.000	1.00	0.00
PRO41	HG2	1.00	0.000	1.00	0.00
PRO41	HD2	1.00	0.000	1.00	0.00
PRO41	HD3	1.00	0.000	1.00	0.00
THR42	H	1.00	0.000	1.00	0.00

**3.41.3 Detailed Probabilities of PRO41CG:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO41	1.00	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	0.008	1.00	0.00
PRO41	HB2	1.00	0.000	1.00	0.00
PRO41	HB3	1.00	0.000	1.00	0.00
PRO41	HG2	1.00	0.000	1.00	0.00
PRO41	HD2	1.00	0.000	1.00	0.00
PRO41	HD3	1.00	0.000	1.00	0.00

**3.41.4 Detailed Probabilities of PRO41CD:**

Overall probability: 0.837

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE40	0.67	1.00
PRO41	1.00	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**

## 3.41 PRO(41)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE40	HA	1.00	0.016	1.00	0.00
PHE40	HB2	0.97	0.069	0.03	0.00
PHE40	HB3	0.98	0.098	0.02	0.00
PHE40	H	0.98	0.002	1.00	0.00
PHE40	HD1	0.74	0.020	1.00	0.00
PHE40	HD2	0.55	0.020	1.00	0.00
PRO41	HA	1.00	0.000	1.00	0.00
PRO41	HB2	1.00	0.000	1.00	0.00
PRO41	HB3	1.00	0.000	1.00	0.00
PRO41	HG2	1.00	0.000	1.00	0.00
PRO41	HD2	1.00	0.000	1.00	0.00
PRO41	HD3	1.00	0.000	1.00	0.00

## 3.41.5 Detailed Probabilities of PRO41HA:

Overall probability: 0.778

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
PHE40	0.00	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	0.293	0.00	0.00
PRO41	HA	1.00	0.000	1.00	0.00
PRO41	HB2	1.00	0.000	1.00	0.00
PRO41	HB3	1.00	0.000	1.00	0.00
PRO41	HG2	1.00	0.008	1.00	0.00
PRO41	HD2	1.00	0.000	1.00	0.00
PRO41	HD3	1.00	0.000	1.00	0.00
THR42	HA	1.00	0.131	0.00	0.00
THR42	H	1.00	0.000	1.00	0.00

**3.41.6 Detailed Probabilities of PRO41HB2:**

Overall probability: 0.877

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO41	1.00	1.00
THR42	0.51	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	0.000	1.00	0.00
PRO41	HB2	1.00	0.000	1.00	0.00
PRO41	HB3	1.00	0.000	1.00	0.00
PRO41	HG2	1.00	0.000	1.00	0.00
PRO41	HD2	1.00	0.000	1.00	0.00
PRO41	HD3	1.00	0.000	1.00	0.00
THR42	HA	0.98	0.817	0.02	0.00
THR42	H	1.00	0.000	1.00	0.00

**3.41.7 Detailed Probabilities of PRO41HB3:**

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	0.000	1.00	0.00
PRO41	HB2	1.00	0.000	1.00	0.00
PRO41	HB3	1.00	0.000	1.00	0.00
PRO41	HG2	1.00	0.000	1.00	0.00
PRO41	HD2	1.00	0.000	1.00	0.00
PRO41	HD3	1.00	0.000	1.00	0.00
THR42	H	1.00	0.000	1.00	0.00

**3.41.8 Detailed Probabilities of PRO41HG2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO41	1.00	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	0.000	1.00	0.00
PRO41	HB2	1.00	0.000	1.00	0.00
PRO41	HB3	1.00	0.000	1.00	0.00
PRO41	HG2	1.00	0.000	1.00	0.00
PRO41	HD2	1.00	0.000	1.00	0.00
PRO41	HD3	1.00	0.000	1.00	0.00

**3.41.9 Detailed Probabilities of PRO41HD2:**

Overall probability: 0.605

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE40	0.26	1.00
PRO41	0.83	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	0.149	0.00	0.00
PHE40	HB2	0.97	0.149	0.03	0.00
PHE40	HB3	0.98	0.149	0.02	0.00
PHE40	H	0.98	0.023	1.00	0.00
PRO41	HA	1.00	0.268	0.00	0.00
PRO41	HB2	1.00	0.000	1.00	0.00
PRO41	HB3	1.00	0.000	1.00	0.00
PRO41	HG2	1.00	0.000	1.00	0.00
PRO41	HD2	1.00	0.000	1.00	0.00
PRO41	HD3	1.00	0.000	1.00	0.00

**3.41.10 Detailed Probabilities of PRO41HD3:**

Overall probability: 0.603

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE40	0.26	1.00
PRO41	0.83	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	0.083	0.00	0.00
PHE40	HB2	0.98	0.083	0.02	0.00
PHE40	HB3	0.99	0.083	0.01	0.00
PHE40	H	0.97	0.005	1.00	0.00
PRO41	HA	1.00	0.500	0.00	0.00
PRO41	HB2	1.00	0.000	1.00	0.00
PRO41	HB3	1.00	0.000	1.00	0.00
PRO41	HG2	1.00	0.000	1.00	0.00
PRO41	HD2	1.00	0.000	1.00	0.00
PRO41	HD3	1.00	0.000	1.00	0.00

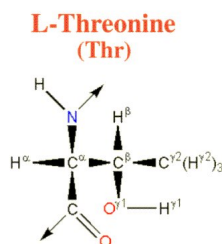
**3.42 THR(42)**

Figure 32: Image from the BMRB

Residue probability: 0.903

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	0.642	0.909
CB 3.42.2	70.881	69.395	4.500	1.000	0.857
CG2 3.42.3	21.440	21.588	1.595	1.000	0.800
N 3.42.4	104.189	115.370	5.913	0.842	0.900
HA 3.42.5	4.980	4.461	0.626	0.820	0.909
HB 3.42.6	4.489	4.172	0.855	1.000	0.857
HG2 3.42.7	1.239	1.134	0.349	1.000	0.800
H 3.42.8	7.123	8.272	1.597	0.917	0.900
HG1	NA	—	—	0.000	0.000

**3.42.1 Detailed Probabilities of THR42CA:**

Overall probability: 0.642

Overall confidence: 0.909

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO41	0.01	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	0.131	0.00	0.00
PRO41	HB2	0.98	0.817	0.02	0.00
THR42	HA	1.00	0.000	1.00	0.00
THR42	HB	1.00	0.000	1.00	0.00
THR42	HG21	1.00	0.000	1.00	0.00
THR42	H	1.00	0.000	1.00	0.00
PRO43	HA	1.00	0.856	0.00	0.00
PRO43	HG2	0.95	0.313	0.05	0.00
PRO43	HD2	1.00	0.022	1.00	0.00
PRO43	HD3	1.00	0.004	1.00	0.00
PRO43	HG3	0.94	0.013	1.00	0.00

**3.42.2 Detailed Probabilities of THR42CB:**

Overall probability: 1.000

Overall confidence: 0.857

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR42	1.00	0.80
PRO43	1.00	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	0.000	1.00	0.00
THR42	HB	1.00	0.000	1.00	0.00
THR42	HG21	1.00	0.000	1.00	0.00
THR42	H	1.00	0.000	1.00	0.00
PRO43	HD2	0.99	0.005	1.00	0.00
PRO43	HD3	0.99	0.004	1.00	0.00

**3.42.3 Detailed Probabilities of THR42CG2:**

Overall probability: 1.000

Overall confidence: 0.800

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR42	1.00	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	0.000	1.00	0.00
THR42	HB	1.00	0.000	1.00	0.00
THR42	HG21	1.00	0.000	1.00	0.00
THR42	H	1.00	0.000	1.00	0.00

**3.42.4 Detailed Probabilities of THR42N:**

Overall probability: 0.842

Overall confidence: 0.900

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO41	1.00	1.00
THR42	1.00	0.80
PRO43	0.05	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	0.000	1.00	0.00
PRO41	HB2	1.00	0.000	1.00	0.00
PRO41	HB3	1.00	0.000	1.00	0.00
PRO41	HG2	0.92	0.000	1.00	0.00
PRO41	HD2	0.67	0.000	1.00	0.00
PRO41	HD3	0.58	0.000	1.00	0.00
THR42	HA	1.00	0.000	1.00	0.00
THR42	HB	1.00	0.000	1.00	0.00
THR42	HG21	1.00	0.000	1.00	0.00
THR42	H	1.00	0.000	1.00	0.00
PRO43	HD2	1.00	0.041	0.00	0.00
PRO43	HD3	0.99	0.039	0.10	0.00

**3.42.5 Detailed Probabilities of THR42HA:**

Overall probability: 0.820

Overall confidence: 0.909

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO41	0.51	1.00
THR42	1.00	0.80
PRO43	0.80	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	0.008	1.00	0.00
PRO41	HB2	0.98	0.360	0.02	0.00
THR42	HA	1.00	0.000	1.00	0.00
THR42	HB	1.00	0.000	1.00	0.00
THR42	HG21	1.00	0.000	1.00	0.00
THR42	H	1.00	0.000	1.00	0.00
PRO43	HA	1.00	1.272	0.00	0.00
PRO43	HG2	0.95	0.005	1.00	0.00
PRO43	HD2	1.00	0.005	1.00	0.00
PRO43	HD3	1.00	0.003	1.00	0.00
PRO43	HG3	0.94	0.003	1.00	0.00

**3.42.6 Detailed Probabilities of THR42HB:**

Overall probability: 1.000

Overall confidence: 0.857

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR42	1.00	0.80
PRO43	1.00	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	0.000	1.00	0.00
THR42	HB	1.00	0.000	1.00	0.00
THR42	HG21	1.00	0.000	1.00	0.00
THR42	H	1.00	0.000	1.00	0.00
PRO43	HD2	0.99	0.001	1.00	0.00
PRO43	HD3	0.99	0.003	1.00	0.00
PRO43	HG2	0.58	0.011	1.00	0.00
PRO43	HG3	0.52	0.007	1.00	0.00

**3.42.7 Detailed Probabilities of THR42HG21:**

Overall probability: 1.000

Overall confidence: 0.800

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR42	1.00	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	0.000	1.00	0.00
THR42	HB	1.00	0.000	1.00	0.00
THR42	HG21	1.00	0.000	1.00	0.00
THR42	H	1.00	0.000	1.00	0.00

**3.42.8 Detailed Probabilities of THR42H:**

Overall probability: 0.917

Overall confidence: 0.900

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO41	1.00	1.00
THR42	1.00	0.80
PRO43	0.50	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	0.000	1.00	0.00
PRO41	HB2	1.00	0.000	1.00	0.00
PRO41	HB3	1.00	0.000	1.00	0.00
PRO41	HG2	0.92	0.000	1.00	0.00
PRO41	HD2	0.67	0.000	1.00	0.00
PRO41	HD3	0.58	0.000	1.00	0.00
THR42	HA	1.00	0.000	1.00	0.00
THR42	HB	1.00	0.000	1.00	0.00
THR42	HG21	1.00	0.000	1.00	0.00
THR42	H	1.00	0.000	1.00	0.00
PRO43	HD2	1.00	0.114	0.00	0.00
PRO43	HD3	0.99	0.000	1.00	0.00

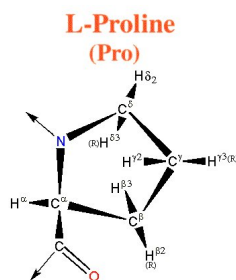


Figure 33: Image from the BMRB

Residue probability: 0.922  
Residue probability confidence: 0.949

**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	0.778	0.900
CB 3.43.2	30.985	33.632	13.629	1.000	0.875
CG 3.43.3	26.838	28.412	13.801	1.000	1.000
CD 3.43.4	50.034	49.797	3.175	1.000	1.000
N	NA	—	—	0.000	0.000
HA 3.43.5	2.776	4.332	0.427	0.778	0.900
HB2 3.43.6	1.664	2.099	0.501	0.878	0.889
HB3 3.43.7	1.818	2.052	0.596	1.000	0.875
HG2 3.43.8	1.982	1.927	0.364	0.881	1.000
HG3 3.43.9	1.656	1.907	0.417	1.000	1.000
HD2 3.43.10	3.708	3.640	0.682	0.910	1.000
HD3 3.43.11	3.628	3.558	0.522	0.918	1.000

**3.43.1 Detailed Probabilities of PRO43CA:**

Overall probability: 0.778  
Overall confidence: 0.900

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR42	0.00	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	1.272	0.00	0.00
PRO43	HA	1.00	0.000	1.00	0.00
PRO43	HB2	1.00	0.000	1.00	0.00
PRO43	HB3	1.00	0.000	1.00	0.00
PRO43	HG2	1.00	0.000	1.00	0.00
PRO43	HG3	1.00	0.000	1.00	0.00
PRO43	HD2	1.00	0.000	1.00	0.00
PRO43	HD3	1.00	0.000	1.00	0.00
ALA44	HA	1.00	0.298	0.00	0.00

**3.43.2 Detailed Probabilities of PRO43CB:**

Overall probability: 1.000

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO43	1.00	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**

## 3.43 PRO(43)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PRO43	HA	1.00	0.000	1.00	0.00
PRO43	HB2	1.00	0.000	1.00	0.00
PRO43	HB3	1.00	0.000	1.00	0.00
PRO43	HG2	1.00	0.000	1.00	0.00
PRO43	HG3	1.00	0.000	1.00	0.00
PRO43	HD2	1.00	0.000	1.00	0.00
PRO43	HD3	1.00	0.000	1.00	0.00

## 3.43.3 Detailed Probabilities of PRO43CG:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
THR42	1.00	1.00
PRO43	1.00	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	0.005	1.00	0.00
THR42	HB	0.58	0.011	1.00	0.00
PRO43	HA	1.00	0.000	1.00	0.00
PRO43	HB2	1.00	0.000	1.00	0.00
PRO43	HB3	1.00	0.000	1.00	0.00
PRO43	HG2	1.00	0.000	1.00	0.00
PRO43	HG3	1.00	0.000	1.00	0.00
PRO43	HD2	1.00	0.000	1.00	0.00
PRO43	HD3	1.00	0.000	1.00	0.00

## 3.43.4 Detailed Probabilities of PRO43CD:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
THR42	1.00	1.00
PRO43	1.00	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	0.00
THR42	HB	0.99	0.003	1.00	0.00
THR42	H	0.99	0.000	1.00	0.00
THR42	HG21	0.79	0.002	1.00	0.00
PRO43	HA	1.00	0.000	1.00	0.00
PRO43	HB2	1.00	0.000	1.00	0.00
PRO43	HB3	1.00	0.000	1.00	0.00
PRO43	HG2	1.00	0.000	1.00	0.00
PRO43	HG3	1.00	0.000	1.00	0.00
PRO43	HD2	1.00	0.000	1.00	0.00
PRO43	HD3	1.00	0.000	1.00	0.00

**3.43.5 Detailed Probabilities of PRO43HA:**

Overall probability: 0.778

Overall confidence: 0.900

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR42	0.00	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	0.856	0.00	0.00
PRO43	HA	1.00	0.000	1.00	0.00
PRO43	HB2	1.00	0.000	1.00	0.00
PRO43	HB3	1.00	0.000	1.00	0.00
PRO43	HG2	1.00	0.000	1.00	0.00
PRO43	HG3	1.00	0.000	1.00	0.00
PRO43	HD2	1.00	0.000	1.00	0.00
PRO43	HD3	1.00	0.000	1.00	0.00
ALA44	HA	1.00	0.346	0.00	0.00

**3.43.6 Detailed Probabilities of PRO43HB2:**

Overall probability: 0.878

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO43	1.00	1.00
ALA44	0.02	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	0.000	1.00	0.00
PRO43	HB2	1.00	0.000	1.00	0.00
PRO43	HB3	1.00	0.000	1.00	0.00
PRO43	HG2	1.00	0.000	1.00	0.00
PRO43	HG3	1.00	0.000	1.00	0.00
PRO43	HD2	1.00	0.000	1.00	0.00
PRO43	HD3	1.00	0.000	1.00	0.00
ALA44	HA	0.98	0.337	0.02	0.00

**3.43.7 Detailed Probabilities of PRO43HB3:**

Overall probability: 1.000

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO43	1.00	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	0.000	1.00	0.00
PRO43	HB2	1.00	0.000	1.00	0.00
PRO43	HB3	1.00	0.000	1.00	0.00
PRO43	HG2	1.00	0.000	1.00	0.00
PRO43	HG3	1.00	0.000	1.00	0.00
PRO43	HD2	1.00	0.000	1.00	0.00
PRO43	HD3	1.00	0.000	1.00	0.00

**3.43.8 Detailed Probabilities of PRO43HG2:**

Overall probability: 0.881

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR42	0.05	1.00
PRO43	1.00	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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR42	HA	0.95	0.313	0.05	0.00
PRO43	HA	1.00	0.000	1.00	0.00
PRO43	HB2	1.00	0.000	1.00	0.00
PRO43	HB3	1.00	0.000	1.00	0.00
PRO43	HG2	1.00	0.000	1.00	0.00
PRO43	HG3	1.00	0.000	1.00	0.00
PRO43	HD2	1.00	0.000	1.00	0.00
PRO43	HD3	1.00	0.000	1.00	0.00

## 3.43.9 Detailed Probabilities of PRO43HG3:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
PRO43	1.00	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	0.000	1.00	0.00
PRO43	HB2	1.00	0.000	1.00	0.00
PRO43	HB3	1.00	0.000	1.00	0.00
PRO43	HG2	1.00	0.000	1.00	0.00
PRO43	HG3	1.00	0.000	1.00	0.00
PRO43	HD2	1.00	0.000	1.00	0.00
PRO43	HD3	1.00	0.000	1.00	0.00

## 3.43.10 Detailed Probabilities of PRO43HD2:

Overall probability: 0.910

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
THR42	0.75	1.00
PRO43	1.00	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	0.022	1.00	0.00
THR42	HB	0.99	0.005	1.00	0.00
THR42	H	1.00	0.041	0.00	0.00
THR42	HG21	0.94	0.021	1.00	0.00
PRO43	HA	1.00	0.000	1.00	0.00
PRO43	HB2	1.00	0.000	1.00	0.00
PRO43	HB3	1.00	0.000	1.00	0.00
PRO43	HG2	1.00	0.000	1.00	0.00
PRO43	HG3	1.00	0.000	1.00	0.00
PRO43	HD2	1.00	0.000	1.00	0.00
PRO43	HD3	1.00	0.000	1.00	0.00

**3.43.11 Detailed Probabilities of PRO43HD3:**

Overall probability: 0.918

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR42	0.78	1.00
PRO43	1.00	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	0.004	1.00	0.00
THR42	HB	0.99	0.004	1.00	0.00
THR42	H	0.99	0.039	0.10	0.00
THR42	HG21	0.79	0.023	1.00	0.00
PRO43	HA	1.00	0.000	1.00	0.00
PRO43	HB2	1.00	0.000	1.00	0.00
PRO43	HB3	1.00	0.000	1.00	0.00
PRO43	HG2	1.00	0.000	1.00	0.00
PRO43	HG3	1.00	0.000	1.00	0.00
PRO43	HD2	1.00	0.000	1.00	0.00
PRO43	HD3	1.00	0.000	1.00	0.00

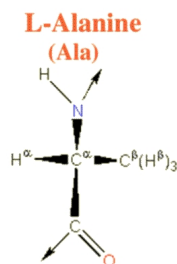
**3.44 ALA(44)**

Figure 34: Image from the BMRB

Residue probability: 0.769

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	0.503	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	0.574	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: 0.503

Overall confidence: 0.857

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO43	0.01	1.00
ALA44	1.00	0.67
ALA45	0.50	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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PRO43	HA	1.00	0.346	0.00	0.00
PRO43	HB2	0.98	0.337	0.02	0.00
ALA44	HA	1.00	0.000	1.00	0.00
ALA44	HB1	1.00	0.000	1.00	0.00
ALA45	HA	1.00	0.460	0.00	0.00
ALA45	H	1.00	0.000	1.00	0.00

## 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	0.000	1.00	0.00
ALA44	HB1	1.00	0.000	1.00	0.00
ALA45	H	1.00	0.000	1.00	0.00
ALA45	HA	0.70	0.006	1.00	0.00

## 3.44.3 Detailed Probabilities of ALA44HA:

Overall probability: 0.574

Overall confidence: 0.857

## Inter- and intra-residue probability

Residue	Probability	Confidence
PRO43	0.34	1.00
ALA44	1.00	0.67
ALA45	0.50	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	0.298	0.00	0.00
PRO43	HB2	0.98	0.298	0.02	0.00
PRO43	HG2	0.60	0.002	1.00	0.00
ALA44	HA	1.00	0.000	1.00	0.00
ALA44	HB1	1.00	0.000	1.00	0.00
ALA45	HA	1.00	0.460	0.00	0.00
ALA45	H	1.00	0.000	1.00	0.00

**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	0.00
ALA44	HB1	1.00	0.000	1.00	0.00
ALA45	H	1.00	0.000	1.00	0.00

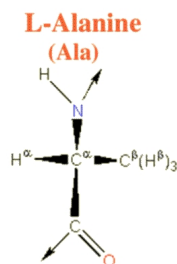
**3.45 ALA(45)**

Figure 35: Image from the BMRB

Residue probability: 0.897

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	0.667	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	0.714	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: 0.667

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ALA44	0.00	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	0.460	0.00	0.00
ALA45	HA	1.00	0.000	1.00	0.00
ALA45	HB1	1.00	0.000	1.00	0.00
ALA45	H	1.00	0.000	1.00	0.00
ALA46	HA	1.00	0.409	0.00	0.00
ALA46	H	1.00	0.000	1.00	0.00

**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	0.00
ALA45	HB1	1.00	0.000	1.00	0.00
ALA45	H	1.00	0.000	1.00	0.00
ALA46	H	1.00	0.000	1.00	0.00
ALA46	HA	0.70	0.005	1.00	0.00

**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	0.000	1.00	0.00
ALA44	HB1	1.00	0.000	1.00	0.00
ALA45	HA	1.00	0.000	1.00	0.00
ALA45	HB1	1.00	0.000	1.00	0.00
ALA45	H	1.00	0.000	1.00	0.00
ALA46	H	1.00	0.000	1.00	0.00

**3.45.4 Detailed Probabilities of ALA45HA:**

Overall probability: 0.714

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ALA44	0.50	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	0.460	0.00	0.00
ALA44	HB1	0.67	0.006	1.00	0.00
ALA45	HA	1.00	0.000	1.00	0.00
ALA45	HB1	1.00	0.000	1.00	0.00
ALA45	H	1.00	0.000	1.00	0.00
ALA46	HA	1.00	0.277	0.00	0.00
ALA46	H	1.00	0.000	1.00	0.00

**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**

## 3.45 ALA(45)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA45	HA	1.00	0.000	1.00	0.00
ALA45	HB1	1.00	0.000	1.00	0.00
ALA45	H	1.00	0.000	1.00	0.00
ALA46	H	1.00	0.000	1.00	0.00
ALA46	HA	0.70	0.017	1.00	0.00

## 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

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA44	HA	1.00	0.000	1.00	0.00
ALA44	HB1	1.00	0.000	1.00	0.00
ALA45	HA	1.00	0.000	1.00	0.00
ALA45	HB1	1.00	0.000	1.00	0.00
ALA45	H	1.00	0.000	1.00	0.00
ALA46	H	1.00	0.000	1.00	0.00
ALA46	HB1	0.52	0.010	1.00	0.00

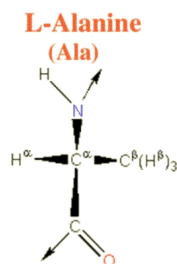
**3.46 ALA(46)**

Figure 36: Image from the BMRB

Residue probability: 0.929

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	0.857	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	0.714	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: 0.857

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ALA45	0.50	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	0.277	0.00	0.00
ALA45	HB1	0.67	0.017	1.00	0.00
ALA46	HA	1.00	0.000	1.00	0.00
ALA46	HB1	1.00	0.000	1.00	0.00
ALA46	H	1.00	0.000	1.00	0.00
PHE47	HA	1.00	0.021	1.00	0.00
PHE47	H	1.00	0.000	1.00	0.00

## 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	0.00
ALA46	HB1	1.00	0.000	1.00	0.00
ALA46	H	1.00	0.000	1.00	0.00
PHE47	H	1.00	0.000	1.00	0.00
PHE47	HA	0.72	0.024	1.00	0.00

## 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	0.000	1.00	0.00
ALA45	HB1	1.00	0.000	1.00	0.00
ALA45	H	1.00	0.000	1.00	0.00
ALA46	HA	1.00	0.000	1.00	0.00
ALA46	HB1	1.00	0.000	1.00	0.00
ALA46	H	1.00	0.000	1.00	0.00
PHE47	H	1.00	0.000	1.00	0.00

**3.46.4 Detailed Probabilities of ALA46HA:**

Overall probability: 0.714

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ALA45	0.50	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	0.409	0.00	0.00
ALA45	HB1	0.67	0.005	1.00	0.00
ALA46	HA	1.00	0.000	1.00	0.00
ALA46	HB1	1.00	0.000	1.00	0.00
ALA46	H	1.00	0.000	1.00	0.00
PHE47	HA	1.00	0.153	0.00	0.00
PHE47	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ALA46	HB1	1.00	0.000	1.00	0.00
ALA46	H	1.00	0.000	1.00	0.00
PHE47	H	1.00	0.000	1.00	0.00
PHE47	HA	0.72	0.005	1.00	0.00

**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	0.000	1.00	0.00
ALA45	HB1	1.00	0.000	1.00	0.00
ALA45	H	1.00	0.000	1.00	0.00
ALA46	HA	1.00	0.000	1.00	0.00
ALA46	HB1	1.00	0.000	1.00	0.00
ALA46	H	1.00	0.000	1.00	0.00
PHE47	H	1.00	0.000	1.00	0.00

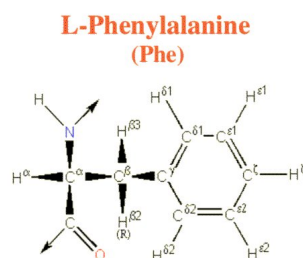


Figure 37: Image from the BMRB

Residue probability: 0.992  
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	0.909	1.000
CB 3.47.2	38.099	40.078	3.616	0.989	1.000
CD1 3.47.3	131.773	131.234	9.579	1.000	1.000
CD2 3.47.4	131.956	131.352	9.581	1.000	1.000
CE1 3.47.5	131.718	130.599	3.219	1.000	1.000
CE2 3.47.6	131.669	130.633	2.839	1.000	1.000
CZ 3.47.7	129.887	129.042	3.448	1.000	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	1.000	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	1.000	1.000
HD1 3.47.12	7.318	7.037	0.347	1.000	1.000
HD2 3.47.13	7.318	7.022	0.417	1.000	1.000
HE1 3.47.14	7.377	7.046	0.417	1.000	1.000
HE2 3.47.15	7.377	7.043	0.400	0.971	1.000
HZ 3.47.16	7.314	6.984	1.598	1.000	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: 0.909  
Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ALA46	0.50	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	0.153	0.00	0.00
ALA46	HB1	0.68	0.005	1.00	0.00
PHE47	HA	1.00	0.000	1.00	0.00
PHE47	HB2	1.00	0.000	1.00	0.00
PHE47	HB3	1.00	0.000	1.00	0.00
PHE47	HD1	1.00	0.003	1.00	0.00
PHE47	HD2	1.00	0.003	1.00	0.00
PHE47	H	1.00	0.000	1.00	0.00
ARG48	HA	1.00	0.006	1.00	0.00
ARG48	H	1.00	0.000	1.00	0.00
ARG48	HB2	0.50	0.006	1.00	0.00

**3.47.2 Detailed Probabilities of PHE47CB:**

Overall probability: 0.989

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE47	0.99	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	0.000	1.00	0.00
PHE47	HB2	1.00	0.000	1.00	0.00
PHE47	HB3	1.00	0.000	1.00	0.00
PHE47	HD1	1.00	0.003	1.00	0.00
PHE47	HD2	1.00	0.003	1.00	0.00
PHE47	HE2	1.00	0.031	0.90	0.00
PHE47	H	1.00	0.000	1.00	0.00
ARG48	H	1.00	0.000	1.00	0.00
ARG48	HA	0.64	0.006	1.00	0.00

## 3.47.3 Detailed Probabilities of PHE47CD1:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
PHE47	1.00	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	0.000	1.00	0.00
PHE47	HB2	1.00	0.000	1.00	0.00
PHE47	HB3	1.00	0.000	1.00	0.00
PHE47	HD1	1.00	0.003	1.00	0.00
PHE47	HD2	1.00	0.003	1.00	0.00
PHE47	HE1	1.00	0.001	1.00	0.00
PHE47	HE2	1.00	0.001	1.00	0.00
PHE47	HZ	1.00	0.000	1.00	0.00
PHE47	H	1.00	0.000	1.00	0.00

## 3.47.4 Detailed Probabilities of PHE47CD2:

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE47	1.00	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	0.000	1.00	0.00
PHE47	HB2	1.00	0.000	1.00	0.00
PHE47	HB3	1.00	0.000	1.00	0.00
PHE47	HD1	1.00	0.003	1.00	0.00
PHE47	HD2	1.00	0.003	1.00	0.00
PHE47	HE1	1.00	0.001	1.00	0.00
PHE47	HE2	1.00	0.001	1.00	0.00
PHE47	HZ	1.00	0.000	1.00	0.00
PHE47	H	0.99	0.000	1.00	0.00

**3.47.5 Detailed Probabilities of PHE47CE1:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE47	1.00	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	0.003	1.00	0.00
PHE47	HD2	1.00	0.003	1.00	0.00
PHE47	HE1	1.00	0.001	1.00	0.00
PHE47	HE2	1.00	0.001	1.00	0.00
PHE47	HZ	1.00	0.000	1.00	0.00
PHE47	HB2	0.90	0.005	1.00	0.00
PHE47	HB3	0.89	0.000	1.00	0.00

**3.47.6 Detailed Probabilities of PHE47CE2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE47	1.00	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	0.005	1.00	0.00
PHE47	HB3	1.00	0.000	1.00	0.00
PHE47	HD1	1.00	0.003	1.00	0.00
PHE47	HD2	1.00	0.003	1.00	0.00
PHE47	HE1	1.00	0.001	1.00	0.00
PHE47	HE2	1.00	0.001	1.00	0.00
PHE47	HZ	1.00	0.000	1.00	0.00

**3.47.7 Detailed Probabilities of PHE47CZ:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE47	1.00	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	0.003	1.00	0.00
PHE47	HD2	1.00	0.003	1.00	0.00
PHE47	HE1	1.00	0.001	1.00	0.00
PHE47	HE2	1.00	0.001	1.00	0.00
PHE47	HZ	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ALA46	HB1	1.00	0.000	1.00	0.00
ALA46	H	1.00	0.000	1.00	0.00
PHE47	HA	1.00	0.000	1.00	0.00
PHE47	HB2	1.00	0.000	1.00	0.00
PHE47	HB3	1.00	0.000	1.00	0.00
PHE47	HD1	1.00	0.028	1.00	0.00
PHE47	HD2	0.99	0.028	1.00	0.00
PHE47	H	1.00	0.000	1.00	0.00
ARG48	H	1.00	0.000	1.00	0.00
ARG48	HA	0.90	0.006	1.00	0.00

**3.47.9 Detailed Probabilities of PHE47HA:**

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
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	0.021	1.00	0.00
ALA46	HB1	0.68	0.024	1.00	0.00
PHE47	HA	1.00	0.000	1.00	0.00
PHE47	HB2	1.00	0.000	1.00	0.00
PHE47	HB3	1.00	0.000	1.00	0.00
PHE47	HD1	1.00	0.000	1.00	0.00
PHE47	HD2	1.00	0.000	1.00	0.00
PHE47	H	1.00	0.000	1.00	0.00
ARG48	HA	1.00	0.006	1.00	0.00
ARG48	H	1.00	0.000	1.00	0.00
ARG48	HB2	0.50	0.006	1.00	0.00

**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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE47	HA	1.00	0.000	1.00	0.00
PHE47	HB2	1.00	0.000	1.00	0.00
PHE47	HB3	1.00	0.000	1.00	0.00
PHE47	HD1	1.00	0.000	1.00	0.00
PHE47	HD2	1.00	0.000	1.00	0.00
PHE47	HE2	1.00	0.005	1.00	0.00
PHE47	H	1.00	0.000	1.00	0.00
PHE47	HE1	0.90	0.005	1.00	0.00
ARG48	H	1.00	0.000	1.00	0.00

## 3.47.11 Detailed Probabilities of PHE47HB3:

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
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	0.000	1.00	0.00
PHE47	HB2	1.00	0.000	1.00	0.00
PHE47	HB3	1.00	0.000	1.00	0.00
PHE47	HD1	1.00	0.000	1.00	0.00
PHE47	HD2	1.00	0.000	1.00	0.00
PHE47	HE2	1.00	0.000	1.00	0.00
PHE47	H	1.00	0.000	1.00	0.00
PHE47	HE1	0.89	0.000	1.00	0.00
ARG48	H	1.00	0.000	1.00	0.00
ARG48	HA	0.85	0.010	1.00	0.00

## 3.47.12 Detailed Probabilities of PHE47HD1:

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE47	1.00	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	0.003	1.00	0.00
PHE47	HB2	1.00	0.003	1.00	0.00
PHE47	HB3	1.00	0.003	1.00	0.00
PHE47	HD1	1.00	0.003	1.00	0.00
PHE47	HD2	1.00	0.003	1.00	0.00
PHE47	HE1	1.00	0.003	1.00	0.00
PHE47	HE2	1.00	0.003	1.00	0.00
PHE47	HZ	1.00	0.003	1.00	0.00
PHE47	H	1.00	0.028	1.00	0.00

**3.47.13 Detailed Probabilities of PHE47HD2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE47	1.00	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	0.003	1.00	0.00
PHE47	HB2	1.00	0.003	1.00	0.00
PHE47	HB3	1.00	0.003	1.00	0.00
PHE47	HD1	1.00	0.003	1.00	0.00
PHE47	HD2	1.00	0.003	1.00	0.00
PHE47	HE1	1.00	0.003	1.00	0.00
PHE47	HE2	1.00	0.003	1.00	0.00
PHE47	HZ	1.00	0.003	1.00	0.00
PHE47	H	0.99	0.028	1.00	0.00

**3.47.14 Detailed Probabilities of PHE47HE1:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE47	1.00	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	0.001	1.00	0.00
PHE47	HD2	1.00	0.001	1.00	0.00
PHE47	HE1	1.00	0.001	1.00	0.00
PHE47	HE2	1.00	0.001	1.00	0.00
PHE47	HZ	1.00	0.001	1.00	0.00

**3.47.15 Detailed Probabilities of PHE47HE2:**

Overall probability: 0.971

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE47	0.97	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	0.031	0.90	0.00
PHE47	HB3	1.00	0.031	0.90	0.00
PHE47	HD1	1.00	0.001	1.00	0.00
PHE47	HD2	1.00	0.001	1.00	0.00
PHE47	HE1	1.00	0.001	1.00	0.00
PHE47	HE2	1.00	0.001	1.00	0.00
PHE47	HZ	1.00	0.001	1.00	0.00

**3.47.16 Detailed Probabilities of PHE47HZ:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE47	1.00	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	0.000	1.00	0.00
PHE47	HD2	1.00	0.000	1.00	0.00
PHE47	HE1	1.00	0.000	1.00	0.00
PHE47	HE2	1.00	0.000	1.00	0.00
PHE47	HZ	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ALA46	HB1	1.00	0.000	1.00	0.00
ALA46	H	1.00	0.000	1.00	0.00
PHE47	HA	1.00	0.000	1.00	0.00
PHE47	HB2	1.00	0.000	1.00	0.00
PHE47	HB3	1.00	0.000	1.00	0.00
PHE47	HD1	1.00	0.000	1.00	0.00
PHE47	HD2	0.99	0.000	1.00	0.00
PHE47	H	1.00	0.000	1.00	0.00
ARG48	H	1.00	0.000	1.00	0.00

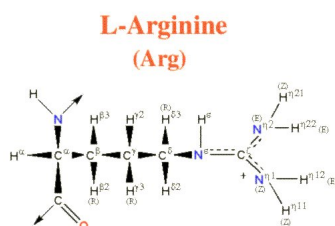


Figure 38: Image from the BMRB

**Residue probability:** 0.986  
**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	0.909	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	1.000	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	0.923	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	1.000	0.889
HG2 3.48.9	1.235	1.559	0.294	1.000	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	1.000	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:** 0.909  
**Overall confidence:** 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE47	1.00	1.00
ARG48	1.00	1.00
SER49	0.50	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	0.006	1.00	0.00
PHE47	HB3	0.85	0.010	1.00	0.00
ARG48	HA	1.00	0.000	1.00	0.00
ARG48	HB2	1.00	0.000	1.00	0.00
ARG48	HB3	1.00	0.000	1.00	0.00
ARG48	HG2	1.00	0.000	1.00	0.00
ARG48	HG3	1.00	0.000	1.00	0.00
ARG48	HD2	0.98	0.000	1.00	0.00
ARG48	H	1.00	0.000	1.00	0.00
SER49	HA	1.00	1.308	0.00	0.00
SER49	H	1.00	0.000	1.00	0.00

**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**

## 3.48 ARG(48)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG48	HA	1.00	0.000	1.00	0.00
ARG48	HB2	1.00	0.000	1.00	0.00
ARG48	HB3	1.00	0.000	1.00	0.00
ARG48	HG2	1.00	0.000	1.00	0.00
ARG48	HG3	1.00	0.000	1.00	0.00
ARG48	HD2	1.00	0.000	1.00	0.00
ARG48	H	1.00	0.000	1.00	0.00
SER49	H	1.00	0.000	1.00	0.00

## 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	0.000	1.00	0.00
ARG48	HB2	1.00	0.000	1.00	0.00
ARG48	HB3	1.00	0.000	1.00	0.00
ARG48	HG2	1.00	0.000	1.00	0.00
ARG48	HG3	1.00	0.000	1.00	0.00
ARG48	HD2	1.00	0.000	1.00	0.00
ARG48	H	1.00	0.000	1.00	0.00
SER49	H	0.97	0.000	1.00	0.00

## 3.48.4 Detailed Probabilities of ARG48CD:

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	0.000	1.00	0.00
ARG48	HB2	1.00	0.000	1.00	0.00
ARG48	HB3	1.00	0.000	1.00	0.00
ARG48	HG2	1.00	0.000	1.00	0.00
ARG48	HG3	1.00	0.000	1.00	0.00
ARG48	HD2	1.00	0.000	1.00	0.00
ARG48	H	0.86	0.000	1.00	0.00

**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	0.000	1.00	0.00
PHE47	HB2	1.00	0.000	1.00	0.00
PHE47	HB3	1.00	0.000	1.00	0.00
PHE47	H	1.00	0.000	1.00	0.00
PHE47	HD1	0.73	0.028	1.00	0.00
PHE47	HD2	0.68	0.028	1.00	0.00
ARG48	HA	1.00	0.000	1.00	0.00
ARG48	HB2	1.00	0.000	1.00	0.00
ARG48	HB3	1.00	0.000	1.00	0.00
ARG48	HG2	1.00	0.000	1.00	0.00
ARG48	HG3	1.00	0.000	1.00	0.00
ARG48	H	1.00	0.000	1.00	0.00
ARG48	HD2	0.87	0.010	1.00	0.00
SER49	H	1.00	0.000	1.00	0.00
SER49	HB2	0.54	0.004	1.00	0.00

**3.48.6 Detailed Probabilities of ARG48HA:**

Overall probability: 0.923

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE47	1.00	1.00
ARG48	1.00	1.00
SER49	0.50	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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE47	HA	1.00	0.006	1.00	0.00
PHE47	HB2	0.64	0.006	1.00	0.00
PHE47	HB3	0.85	0.006	1.00	0.00
PHE47	H	0.90	0.006	1.00	0.00
ARG48	HA	1.00	0.000	1.00	0.00
ARG48	HB2	1.00	0.000	1.00	0.00
ARG48	HB3	1.00	0.000	1.00	0.00
ARG48	HG2	1.00	0.000	1.00	0.00
ARG48	HG3	1.00	0.000	1.00	0.00
ARG48	HD2	0.98	0.000	1.00	0.00
ARG48	H	1.00	0.000	1.00	0.00
SER49	HA	1.00	0.258	0.00	0.00
SER49	H	1.00	0.000	1.00	0.00

## 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	0.000	1.00	0.00
ARG48	HB2	1.00	0.000	1.00	0.00
ARG48	HB3	1.00	0.000	1.00	0.00
ARG48	HG2	1.00	0.000	1.00	0.00
ARG48	HG3	1.00	0.000	1.00	0.00
ARG48	HD2	1.00	0.000	1.00	0.00
ARG48	H	1.00	0.000	1.00	0.00
SER49	H	1.00	0.000	1.00	0.00

**3.48.8 Detailed Probabilities of ARG48HB3:**

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
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	0.000	1.00	0.00
ARG48	HB2	1.00	0.000	1.00	0.00
ARG48	HB3	1.00	0.000	1.00	0.00
ARG48	HG2	1.00	0.000	1.00	0.00
ARG48	HG3	1.00	0.000	1.00	0.00
ARG48	HD2	1.00	0.000	1.00	0.00
ARG48	H	1.00	0.000	1.00	0.00
SER49	H	1.00	0.000	1.00	0.00

**3.48.9 Detailed Probabilities of ARG48HG2:**

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	0.000	1.00	0.00
ARG48	HB2	1.00	0.000	1.00	0.00
ARG48	HB3	1.00	0.000	1.00	0.00
ARG48	HG2	1.00	0.000	1.00	0.00
ARG48	HG3	1.00	0.000	1.00	0.00
ARG48	HD2	1.00	0.000	1.00	0.00
ARG48	H	1.00	0.000	1.00	0.00
SER49	H	0.97	0.000	1.00	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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG48	HA	1.00	0.000	1.00	0.00
ARG48	HB2	1.00	0.000	1.00	0.00
ARG48	HB3	1.00	0.000	1.00	0.00
ARG48	HG2	1.00	0.000	1.00	0.00
ARG48	HG3	1.00	0.000	1.00	0.00
ARG48	HD2	1.00	0.000	1.00	0.00
ARG48	H	1.00	0.000	1.00	0.00
SER49	H	0.96	0.000	1.00	0.00

## 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	0.000	1.00	0.00
ARG48	HB2	1.00	0.000	1.00	0.00
ARG48	HB3	1.00	0.000	1.00	0.00
ARG48	HG2	1.00	0.000	1.00	0.00
ARG48	HG3	1.00	0.000	1.00	0.00
ARG48	HD2	1.00	0.000	1.00	0.00
ARG48	H	0.86	0.010	1.00	0.00

## 3.48.12 Detailed Probabilities of ARG48H:

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	0.000	1.00	0.00
PHE47	HB2	1.00	0.000	1.00	0.00
PHE47	HB3	1.00	0.000	1.00	0.00
PHE47	H	1.00	0.000	1.00	0.00
PHE47	HD1	0.73	0.000	1.00	0.00
PHE47	HD2	0.68	0.000	1.00	0.00
ARG48	HA	1.00	0.000	1.00	0.00
ARG48	HB2	1.00	0.000	1.00	0.00
ARG48	HB3	1.00	0.000	1.00	0.00
ARG48	HG2	1.00	0.000	1.00	0.00
ARG48	HG3	1.00	0.000	1.00	0.00
ARG48	H	1.00	0.000	1.00	0.00
ARG48	HD2	0.87	0.000	1.00	0.00
SER49	H	1.00	0.000	1.00	0.00
SER49	HB2	0.54	0.027	1.00	0.00

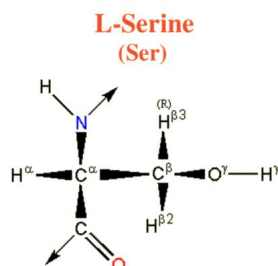
**3.49 SER(49)**

Figure 39: Image from the BMRB

Residue probability: 0.769

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	0.700	0.889
CB 3.49.2	65.466	63.523	4.288	0.677	0.857
N 3.49.3	111.050	116.135	5.326	0.931	0.923
HA 3.49.4	5.524	4.486	0.430	0.800	0.889
HB2 3.49.5	3.230	3.856	0.325	0.677	0.857
HB3 3.49.6	3.823	3.825	0.343	0.839	0.857
H 3.49.7	7.711	8.292	0.600	0.759	0.923
HG	NA	—	—	0.000	0.000

**3.49.1 Detailed Probabilities of SER49CA:**

Overall probability: 0.700

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ARG48	0.00	1.00
SER49	1.00	0.80
PRO50	0.60	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	0.258	0.00	0.00
SER49	HA	1.00	0.000	1.00	0.00
SER49	HB2	1.00	0.000	1.00	0.00
SER49	HB3	1.00	0.000	1.00	0.00
SER49	H	1.00	0.000	1.00	0.00
PRO50	HA	1.00	0.236	0.00	0.00
PRO50	HD2	1.00	0.012	1.00	0.00
PRO50	HD3	1.00	0.040	0.00	0.00
PRO50	HG2	0.94	0.012	1.00	0.00
PRO50	HG3	0.89	0.015	1.00	0.00

**3.49.2 Detailed Probabilities of SER49CB:**

Overall probability: 0.677

Overall confidence: 0.857

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER49	1.00	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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER49	HA	1.00	0.000	1.00	0.00
SER49	HB2	1.00	0.000	1.00	0.00
SER49	HB3	1.00	0.000	1.00	0.00
SER49	H	1.00	0.000	1.00	0.00
PRO50	HD2	0.96	0.147	0.04	0.00
PRO50	HD3	0.98	0.040	0.02	0.00

**3.49.3 Detailed Probabilities of SER49N:**

Overall probability: 0.931

Overall confidence: 0.923

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ARG48	1.00	1.00
SER49	1.00	0.80
PRO50	0.68	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	0.000	1.00	0.00
ARG48	HB2	1.00	0.000	1.00	0.00
ARG48	HB3	1.00	0.000	1.00	0.00
ARG48	HG2	0.97	0.000	1.00	0.00
ARG48	HG3	0.96	0.000	1.00	0.00
ARG48	H	1.00	0.000	1.00	0.00
ARG48	HD2	0.55	0.000	1.00	0.00
SER49	HA	1.00	0.000	1.00	0.00
SER49	HB2	1.00	0.000	1.00	0.00
SER49	HB3	1.00	0.000	1.00	0.00
SER49	H	1.00	0.000	1.00	0.00
PRO50	HD2	0.98	0.012	1.00	0.00
PRO50	HD3	0.96	0.040	0.04	0.00
PRO50	HA	0.65	0.022	1.00	0.00

**3.49.4 Detailed Probabilities of SER49HA:**

Overall probability: 0.800

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ARG48	0.00	1.00
SER49	1.00	0.80
PRO50	0.80	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	1.308	0.00	0.00
SER49	HA	1.00	0.000	1.00	0.00
SER49	HB2	1.00	0.000	1.00	0.00
SER49	HB3	1.00	0.000	1.00	0.00
SER49	H	1.00	0.000	1.00	0.00
PRO50	HA	1.00	0.914	0.00	0.00
PRO50	HD2	1.00	0.008	1.00	0.00
PRO50	HD3	1.00	0.004	1.00	0.00
PRO50	HG2	0.94	0.004	1.00	0.00
PRO50	HG3	0.89	0.004	1.00	0.00

**3.49.5 Detailed Probabilities of SER49HB2:**

Overall probability: 0.677

Overall confidence: 0.857

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER49	1.00	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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER49	HA	1.00	0.000	1.00	0.00
SER49	HB2	1.00	0.000	1.00	0.00
SER49	HB3	1.00	0.000	1.00	0.00
SER49	H	1.00	0.000	1.00	0.00
PRO50	HD2	0.96	0.315	0.04	0.00
PRO50	HD3	0.98	0.386	0.02	0.00

**3.49.6 Detailed Probabilities of SER49HB3:**

Overall probability: 0.839

Overall confidence: 0.857

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER49	1.00	0.80
PRO50	0.52	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	0.000	1.00	0.00
SER49	HB2	1.00	0.000	1.00	0.00
SER49	HB3	1.00	0.000	1.00	0.00
SER49	H	1.00	0.000	1.00	0.00
PRO50	HD2	0.97	0.040	0.03	0.00
PRO50	HD3	0.99	0.022	1.00	0.00

**3.49.7 Detailed Probabilities of SER49H:**

Overall probability: 0.759

Overall confidence: 0.923

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ARG48	0.84	1.00
SER49	1.00	0.80
PRO50	0.03	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	0.000	1.00	0.00
ARG48	HB2	1.00	0.000	1.00	0.00
ARG48	HB3	1.00	0.000	1.00	0.00
ARG48	HG2	0.97	0.000	1.00	0.00
ARG48	HG3	0.96	0.361	0.04	0.00
ARG48	H	1.00	0.000	1.00	0.00
SER49	HA	1.00	0.000	1.00	0.00
SER49	HB2	1.00	0.000	1.00	0.00
SER49	HB3	1.00	0.000	1.00	0.00
SER49	H	1.00	0.000	1.00	0.00
PRO50	HD2	0.98	0.728	0.02	0.00
PRO50	HD3	0.96	0.995	0.04	0.00

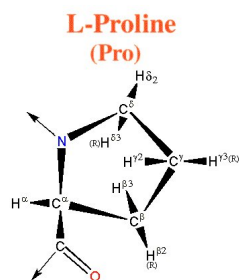


Figure 40: Image from the BMRB

**Residue probability:** 0.910  
**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	0.900	1.000
CB 3.50.2	32.122	33.632	13.629	1.000	1.000
CG 3.50.3	27.711	28.412	13.801	1.000	1.000
CD 3.50.4	50.987	49.797	3.175	0.823	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	1.000	1.000
HB3 3.50.7	2.549	2.052	0.596	1.000	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	1.000	1.000
HD2 3.50.10	3.970	3.640	0.682	0.825	1.000
HD3 3.50.11	3.863	3.558	0.522	0.643	1.000

**3.50.1 Detailed Probabilities of PRO50CA:**

**Overall probability:** 0.900  
**Overall confidence:** 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER49	0.00	1.00
PRO50	1.00	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	0.914	0.00	0.00
PRO50	HA	1.00	0.000	1.00	0.00
PRO50	HB2	1.00	0.000	1.00	0.00
PRO50	HB3	1.00	0.000	1.00	0.00
PRO50	HG2	1.00	0.000	1.00	0.00
PRO50	HG3	1.00	0.000	1.00	0.00
PRO50	HD2	1.00	0.000	1.00	0.00
PRO50	HD3	1.00	0.000	1.00	0.00
LEU51	HA	1.00	0.004	1.00	0.00
LEU51	H	1.00	0.000	1.00	0.00

**3.50.2 Detailed Probabilities of PRO50CB:**

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

**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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PRO50	HA	1.00	0.000	1.00	0.00
PRO50	HB2	1.00	0.000	1.00	0.00
PRO50	HB3	1.00	0.000	1.00	0.00
PRO50	HG2	1.00	0.000	1.00	0.00
PRO50	HG3	1.00	0.000	1.00	0.00
PRO50	HD2	1.00	0.000	1.00	0.00
PRO50	HD3	1.00	0.000	1.00	0.00
LEU51	H	1.00	0.000	1.00	0.00

## 3.50.3 Detailed Probabilities of PRO50CG:

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	0.000	1.00	0.00
PRO50	HB2	1.00	0.000	1.00	0.00
PRO50	HB3	1.00	0.000	1.00	0.00
PRO50	HG2	1.00	0.000	1.00	0.00
PRO50	HG3	1.00	0.000	1.00	0.00
PRO50	HD2	1.00	0.000	1.00	0.00
PRO50	HD3	1.00	0.000	1.00	0.00

## 3.50.4 Detailed Probabilities of PRO50CD:

Overall probability: 0.823

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
SER49	0.51	1.00
PRO50	1.00	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	0.004	1.00	0.00
SER49	HB2	0.98	0.386	0.02	0.00
SER49	HB3	0.99	0.022	1.00	0.00
SER49	H	0.96	0.995	0.04	0.00
PRO50	HA	1.00	0.000	1.00	0.00
PRO50	HB2	1.00	0.000	1.00	0.00
PRO50	HB3	1.00	0.000	1.00	0.00
PRO50	HG2	1.00	0.000	1.00	0.00
PRO50	HG3	1.00	0.000	1.00	0.00
PRO50	HD2	1.00	0.000	1.00	0.00
PRO50	HD3	1.00	0.000	1.00	0.00

**3.50.5 Detailed Probabilities of PRO50HA:**

Overall probability: 0.818

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER49	0.50	1.00
PRO50	1.00	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	0.236	0.00	0.00
SER49	H	0.65	0.022	1.00	0.00
PRO50	HA	1.00	0.000	1.00	0.00
PRO50	HB2	1.00	0.000	1.00	0.00
PRO50	HB3	1.00	0.000	1.00	0.00
PRO50	HG2	1.00	0.000	1.00	0.00
PRO50	HG3	1.00	0.000	1.00	0.00
PRO50	HD2	1.00	0.000	1.00	0.00
PRO50	HD3	1.00	0.000	1.00	0.00
LEU51	HA	1.00	0.193	0.00	0.00
LEU51	H	1.00	0.000	1.00	0.00

**3.50.6 Detailed Probabilities of PRO50HB2:**

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

**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	0.000	1.00	0.00
PRO50	HB2	1.00	0.000	1.00	0.00
PRO50	HB3	1.00	0.000	1.00	0.00
PRO50	HG2	1.00	0.000	1.00	0.00
PRO50	HG3	1.00	0.000	1.00	0.00
PRO50	HD2	1.00	0.000	1.00	0.00
PRO50	HD3	1.00	0.000	1.00	0.00
LEU51	HA	0.99	0.025	1.00	0.00
LEU51	H	1.00	0.000	1.00	0.00

**3.50.7 Detailed Probabilities of PRO50HB3:**

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

**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	0.00
PRO50	HB2	1.00	0.000	1.00	0.00
PRO50	HB3	1.00	0.000	1.00	0.00
PRO50	HG2	1.00	0.000	1.00	0.00
PRO50	HG3	1.00	0.000	1.00	0.00
PRO50	HD2	1.00	0.000	1.00	0.00
PRO50	HD3	1.00	0.000	1.00	0.00
LEU51	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
PRO50	HB2	1.00	0.000	1.00	0.00
PRO50	HB3	1.00	0.000	1.00	0.00
PRO50	HG2	1.00	0.000	1.00	0.00
PRO50	HG3	1.00	0.000	1.00	0.00
PRO50	HD2	1.00	0.000	1.00	0.00
PRO50	HD3	1.00	0.000	1.00	0.00

**3.50.9 Detailed Probabilities of PRO50HG3:**

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
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	0.000	1.00	0.00
PRO50	HB2	1.00	0.000	1.00	0.00
PRO50	HB3	1.00	0.000	1.00	0.00
PRO50	HG2	1.00	0.000	1.00	0.00
PRO50	HG3	1.00	0.000	1.00	0.00
PRO50	HD2	1.00	0.000	1.00	0.00
PRO50	HD3	1.00	0.000	1.00	0.00

**3.50.10 Detailed Probabilities of PRO50HD2:**

Overall probability: 0.825

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER49	0.52	1.00
PRO50	1.00	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	0.012	1.00	0.00
SER49	HB2	0.96	0.147	0.04	0.00
SER49	HB3	0.97	0.147	0.03	0.00
SER49	H	0.98	0.012	1.00	0.00
PRO50	HA	1.00	0.000	1.00	0.00
PRO50	HB2	1.00	0.000	1.00	0.00
PRO50	HB3	1.00	0.000	1.00	0.00
PRO50	HG2	1.00	0.000	1.00	0.00
PRO50	HG3	1.00	0.000	1.00	0.00
PRO50	HD2	1.00	0.000	1.00	0.00
PRO50	HD3	1.00	0.000	1.00	0.00

**3.50.11 Detailed Probabilities of PRO50HD3:**

Overall probability: 0.643

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER49	0.02	1.00
PRO50	1.00	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	0.040	0.00	0.00
SER49	HB2	0.98	0.040	0.02	0.00
SER49	HB3	0.99	0.040	0.01	0.00
SER49	H	0.96	0.040	0.04	0.00
PRO50	HA	1.00	0.000	1.00	0.00
PRO50	HB2	1.00	0.000	1.00	0.00
PRO50	HB3	1.00	0.000	1.00	0.00
PRO50	HG2	1.00	0.000	1.00	0.00
PRO50	HG3	1.00	0.000	1.00	0.00
PRO50	HD2	1.00	0.000	1.00	0.00
PRO50	HD3	1.00	0.000	1.00	0.00

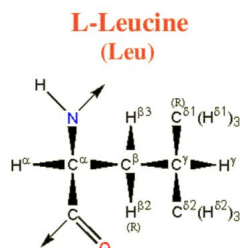


Figure 41: Image from the BMRB

Residue probability: 0.972  
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	0.818	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	1.000	1.000
CD1 3.51.4	22.156	24.837	3.657	1.000	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	0.819	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	1.000	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: 0.818  
Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO50	0.50	1.00
LEU51	1.00	1.00
ALA52	0.50	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	0.193	0.00	0.00
PRO50	HB2	0.99	0.025	1.00	0.00
LEU51	HA	1.00	0.000	1.00	0.00
LEU51	HB2	1.00	0.000	1.00	0.00
LEU51	HB3	1.00	0.000	1.00	0.00
LEU51	HG	1.00	0.000	1.00	0.00
LEU51	HD11	0.99	0.000	1.00	0.00
LEU51	HD21	0.99	0.000	1.00	0.00
LEU51	H	1.00	0.000	1.00	0.00
ALA52	HA	1.00	0.042	0.00	0.00
ALA52	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
LEU51	HB2	1.00	0.000	1.00	0.00
LEU51	HB3	1.00	0.000	1.00	0.00
LEU51	HG	1.00	0.000	1.00	0.00
LEU51	HD11	1.00	0.000	1.00	0.00
LEU51	HD21	1.00	0.000	1.00	0.00
LEU51	H	1.00	0.000	1.00	0.00
ALA52	H	1.00	0.000	1.00	0.00

## 3.51.3 Detailed Probabilities of LEU51CG:

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
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	0.000	1.00	0.00
LEU51	HB2	1.00	0.000	1.00	0.00
LEU51	HB3	1.00	0.000	1.00	0.00
LEU51	HG	1.00	0.000	1.00	0.00
LEU51	HD11	1.00	0.000	1.00	0.00
LEU51	HD21	1.00	0.000	1.00	0.00
LEU51	H	1.00	0.000	1.00	0.00
ALA52	H	0.98	0.000	1.00	0.00

## 3.51.4 Detailed Probabilities of LEU51CD1:

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	0.000	1.00	0.00
LEU51	HB2	1.00	0.000	1.00	0.00
LEU51	HB3	1.00	0.000	1.00	0.00
LEU51	HG	1.00	0.000	1.00	0.00
LEU51	HD11	1.00	0.000	1.00	0.00
LEU51	HD21	1.00	0.000	1.00	0.00
LEU51	H	0.86	0.000	1.00	0.00

**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	0.000	1.00	0.00
LEU51	HB2	1.00	0.000	1.00	0.00
LEU51	HB3	1.00	0.000	1.00	0.00
LEU51	HG	1.00	0.000	1.00	0.00
LEU51	HD11	1.00	0.000	1.00	0.00
LEU51	HD21	1.00	0.000	1.00	0.00
LEU51	H	0.85	0.000	1.00	0.00

**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	0.000	1.00	0.00
PRO50	HB2	1.00	0.000	1.00	0.00
PRO50	HB3	1.00	0.000	1.00	0.00
PRO50	HG2	0.91	0.000	1.00	0.00
PRO50	HG3	0.74	0.000	1.00	0.00
PRO50	HD2	0.67	0.000	1.00	0.00
PRO50	HD3	0.57	0.000	1.00	0.00
LEU51	HA	1.00	0.000	1.00	0.00
LEU51	HB2	1.00	0.000	1.00	0.00
LEU51	HB3	1.00	0.000	1.00	0.00
LEU51	HG	1.00	0.000	1.00	0.00
LEU51	H	1.00	0.000	1.00	0.00
LEU51	HD11	0.88	0.000	1.00	0.00
LEU51	HD21	0.87	0.000	1.00	0.00
ALA52	H	1.00	0.000	1.00	0.00

**3.51.7 Detailed Probabilities of LEU51HA:**

Overall probability: 0.819

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO50	0.51	1.00
LEU51	1.00	1.00
ALA52	0.50	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	0.004	1.00	0.00
PRO50	HB2	0.99	0.200	0.01	0.00
LEU51	HA	1.00	0.000	1.00	0.00
LEU51	HB2	1.00	0.000	1.00	0.00
LEU51	HB3	1.00	0.000	1.00	0.00
LEU51	HG	1.00	0.000	1.00	0.00
LEU51	HD11	0.99	0.000	1.00	0.00
LEU51	HD21	0.99	0.000	1.00	0.00
LEU51	H	1.00	0.000	1.00	0.00
ALA52	HA	1.00	0.042	0.00	0.00
ALA52	H	1.00	0.000	1.00	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	0.000	1.00	0.00
LEU51	HB2	1.00	0.000	1.00	0.00
LEU51	HB3	1.00	0.000	1.00	0.00
LEU51	HG	1.00	0.000	1.00	0.00
LEU51	HD11	1.00	0.000	1.00	0.00
LEU51	HD21	1.00	0.000	1.00	0.00
LEU51	H	1.00	0.000	1.00	0.00
ALA52	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
LEU51	HB2	1.00	0.000	1.00	0.00
LEU51	HB3	1.00	0.000	1.00	0.00
LEU51	HG	1.00	0.000	1.00	0.00
LEU51	HD11	1.00	0.000	1.00	0.00
LEU51	HD21	1.00	0.000	1.00	0.00
LEU51	H	1.00	0.000	1.00	0.00
ALA52	H	1.00	0.000	1.00	0.00
ALA52	HA	0.92	0.028	1.00	0.00

**3.51.10 Detailed Probabilities of LEU51HG:**

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
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	0.000	1.00	0.00
LEU51	HB2	1.00	0.000	1.00	0.00
LEU51	HB3	1.00	0.000	1.00	0.00
LEU51	HG	1.00	0.000	1.00	0.00
LEU51	HD11	1.00	0.000	1.00	0.00
LEU51	HD21	1.00	0.000	1.00	0.00
LEU51	H	1.00	0.000	1.00	0.00
ALA52	H	0.98	0.000	1.00	0.00

**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	0.000	1.00	0.00
LEU51	HB2	1.00	0.000	1.00	0.00
LEU51	HB3	1.00	0.000	1.00	0.00
LEU51	HG	1.00	0.000	1.00	0.00
LEU51	HD11	1.00	0.000	1.00	0.00
LEU51	HD21	1.00	0.000	1.00	0.00
LEU51	H	0.86	0.000	1.00	0.00

**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	0.000	1.00	0.00
LEU51	HB2	1.00	0.000	1.00	0.00
LEU51	HB3	1.00	0.000	1.00	0.00
LEU51	HG	1.00	0.000	1.00	0.00
LEU51	HD11	1.00	0.000	1.00	0.00
LEU51	HD21	1.00	0.000	1.00	0.00
LEU51	H	0.85	0.000	1.00	0.00

**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	0.00
PRO50	HB2	1.00	0.000	1.00	0.00
PRO50	HB3	1.00	0.000	1.00	0.00
PRO50	HG2	0.91	0.000	1.00	0.00
PRO50	HG3	0.74	0.000	1.00	0.00
PRO50	HD2	0.67	0.000	1.00	0.00
PRO50	HD3	0.57	0.000	1.00	0.00
LEU51	HA	1.00	0.000	1.00	0.00
LEU51	HB2	1.00	0.000	1.00	0.00
LEU51	HB3	1.00	0.000	1.00	0.00
LEU51	HG	1.00	0.000	1.00	0.00
LEU51	H	1.00	0.000	1.00	0.00
LEU51	HD11	0.88	0.000	1.00	0.00
LEU51	HD21	0.87	0.000	1.00	0.00
ALA52	H	1.00	0.000	1.00	0.00

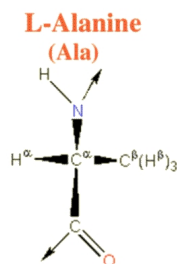
**3.52 ALA(52)**

Figure 42: 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
CA 3.52.1	55.692	53.289	3.425	0.714	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	1.000	1.000
HA 3.52.4	3.621	4.254	0.459	0.667	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: 0.714

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU51	0.50	1.00
ALA52	1.00	1.00
ARG53	0.50	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	0.042	0.00	0.00
LEU51	HB3	0.92	0.028	1.00	0.00
ALA52	HA	1.00	0.000	1.00	0.00
ALA52	HB1	1.00	0.000	1.00	0.00
ALA52	H	1.00	0.000	1.00	0.00
ARG53	HA	1.00	0.179	0.00	0.00
ARG53	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ALA52	HB1	1.00	0.000	1.00	0.00
ALA52	H	1.00	0.000	1.00	0.00
ARG53	H	1.00	0.000	1.00	0.00
ARG53	HA	0.69	0.020	1.00	0.00

**3.52.3 Detailed Probabilities of ALA52N:**

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	0.000	1.00	0.00
LEU51	HB2	1.00	0.000	1.00	0.00
LEU51	HB3	1.00	0.000	1.00	0.00
LEU51	HG	0.98	0.000	1.00	0.00
LEU51	H	1.00	0.000	1.00	0.00
LEU51	HD11	0.53	0.000	1.00	0.00
LEU51	HD21	0.58	0.000	1.00	0.00
ALA52	HA	1.00	0.000	1.00	0.00
ALA52	HB1	1.00	0.000	1.00	0.00
ALA52	H	1.00	0.000	1.00	0.00
ARG53	H	1.00	0.000	1.00	0.00
ARG53	HA	0.87	0.012	1.00	0.00

**3.52.4 Detailed Probabilities of ALA52HA:**

Overall probability: 0.667

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU51	0.00	1.00
ALA52	1.00	1.00
ARG53	0.50	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	0.042	0.00	0.00
ALA52	HA	1.00	0.000	1.00	0.00
ALA52	HB1	1.00	0.000	1.00	0.00
ALA52	H	1.00	0.000	1.00	0.00
ARG53	HA	1.00	0.179	0.00	0.00
ARG53	H	1.00	0.000	1.00	0.00

## 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	0.000	1.00	0.00
ALA52	HB1	1.00	0.000	1.00	0.00
ALA52	H	1.00	0.000	1.00	0.00
ARG53	H	1.00	0.000	1.00	0.00
ARG53	HA	0.69	0.009	1.00	0.00

## 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	0.000	1.00	0.00
LEU51	HB2	1.00	0.000	1.00	0.00
LEU51	HB3	1.00	0.000	1.00	0.00
LEU51	HG	0.98	0.000	1.00	0.00
LEU51	H	1.00	0.000	1.00	0.00
LEU51	HD11	0.53	0.000	1.00	0.00
LEU51	HD21	0.58	0.000	1.00	0.00
ALA52	HA	1.00	0.000	1.00	0.00
ALA52	HB1	1.00	0.000	1.00	0.00
ALA52	H	1.00	0.000	1.00	0.00
ARG53	H	1.00	0.000	1.00	0.00

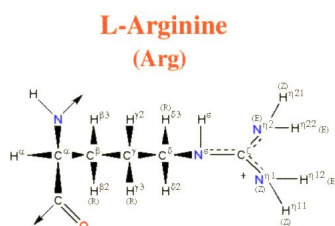


Figure 43: Image from the BMRB

Residue probability: 0.975  
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	0.833	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	1.000	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	0.846	1.000
HB2 3.53.7	1.938	1.793	0.292	1.000	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	1.000	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	1.000	0.700
HD3 3.53.12	3.104	3.081	0.306	1.000	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: 0.833  
Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ALA52	0.50	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	0.179	0.00	0.00
ALA52	HB1	0.67	0.009	1.00	0.00
ARG53	HA	1.00	0.000	1.00	0.00
ARG53	HB2	1.00	0.000	1.00	0.00
ARG53	HB3	1.00	0.000	1.00	0.00
ARG53	HG2	1.00	0.000	1.00	0.00
ARG53	HG3	1.00	0.000	1.00	0.00
ARG53	HD2	0.98	0.000	1.00	0.00
ARG53	HD3	0.97	0.000	1.00	0.00
ARG53	H	1.00	0.000	1.00	0.00
GLN54	HA	1.00	0.201	0.00	0.00
GLN54	H	1.00	0.000	1.00	0.00

**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
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	0.000	1.00	0.00
ARG53	HB2	1.00	0.000	1.00	0.00
ARG53	HB3	1.00	0.000	1.00	0.00
ARG53	HG2	1.00	0.000	1.00	0.00
ARG53	HG3	1.00	0.000	1.00	0.00
ARG53	HD2	1.00	0.000	1.00	0.00
ARG53	HD3	1.00	0.000	1.00	0.00
ARG53	H	1.00	0.000	1.00	0.00
GLN54	H	1.00	0.000	1.00	0.00

**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
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	0.000	1.00	0.00
ARG53	HB2	1.00	0.000	1.00	0.00
ARG53	HB3	1.00	0.000	1.00	0.00
ARG53	HG2	1.00	0.000	1.00	0.00
ARG53	HG3	1.00	0.000	1.00	0.00
ARG53	HD2	1.00	0.000	1.00	0.00
ARG53	HD3	1.00	0.000	1.00	0.00
ARG53	H	1.00	0.000	1.00	0.00
GLN54	H	0.97	0.000	1.00	0.00

**3.53.4 Detailed Probabilities of ARG53CD:**

Overall probability: 1.000

Overall confidence: 0.700

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ARG53	1.00	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	0.00
ARG53	HB2	1.00	0.000	1.00	0.00
ARG53	HB3	1.00	0.000	1.00	0.00
ARG53	HG2	1.00	0.000	1.00	0.00
ARG53	HG3	1.00	0.000	1.00	0.00
ARG53	HD2	1.00	0.000	1.00	0.00
ARG53	HD3	1.00	0.000	1.00	0.00
ARG53	H	0.87	0.000	1.00	0.00

**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	0.00
ALA52	HB1	1.00	0.000	1.00	0.00
ALA52	H	1.00	0.000	1.00	0.00
ARG53	HA	1.00	0.000	1.00	0.00
ARG53	HB2	1.00	0.000	1.00	0.00
ARG53	HB3	1.00	0.000	1.00	0.00
ARG53	HG2	1.00	0.000	1.00	0.00
ARG53	HG3	1.00	0.000	1.00	0.00
ARG53	H	1.00	0.000	1.00	0.00
ARG53	HD2	0.87	0.000	1.00	0.00
ARG53	HD3	0.86	0.000	1.00	0.00
GLN54	H	1.00	0.000	1.00	0.00
GLN54	HB2	0.61	0.003	1.00	0.00

**3.53.6 Detailed Probabilities of ARG53HA:**

Overall probability: 0.846

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ALA52	0.67	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	0.179	0.00	0.00
ALA52	HB1	0.67	0.020	1.00	0.00
ALA52	H	0.87	0.012	1.00	0.00
ARG53	HA	1.00	0.000	1.00	0.00
ARG53	HB2	1.00	0.000	1.00	0.00
ARG53	HB3	1.00	0.000	1.00	0.00
ARG53	HG2	1.00	0.000	1.00	0.00
ARG53	HG3	1.00	0.000	1.00	0.00
ARG53	HD2	0.98	0.000	1.00	0.00
ARG53	HD3	0.97	0.000	1.00	0.00
ARG53	H	1.00	0.000	1.00	0.00
GLN54	HA	1.00	0.201	0.00	0.00
GLN54	H	1.00	0.000	1.00	0.00

**3.53.7 Detailed Probabilities of ARG53HB2:**

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
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	0.000	1.00	0.00
ARG53	HB2	1.00	0.000	1.00	0.00
ARG53	HB3	1.00	0.000	1.00	0.00
ARG53	HG2	1.00	0.000	1.00	0.00
ARG53	HG3	1.00	0.000	1.00	0.00
ARG53	HD2	1.00	0.000	1.00	0.00
ARG53	HD3	1.00	0.000	1.00	0.00
ARG53	H	1.00	0.000	1.00	0.00
GLN54	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ARG53	HB2	1.00	0.000	1.00	0.00
ARG53	HB3	1.00	0.000	1.00	0.00
ARG53	HG2	1.00	0.000	1.00	0.00
ARG53	HG3	1.00	0.000	1.00	0.00
ARG53	HD2	1.00	0.000	1.00	0.00
ARG53	HD3	1.00	0.000	1.00	0.00
ARG53	H	1.00	0.000	1.00	0.00
GLN54	H	1.00	0.000	1.00	0.00

**3.53.9 Detailed Probabilities of ARG53HG2:**

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
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	0.000	1.00	0.00
ARG53	HB2	1.00	0.000	1.00	0.00
ARG53	HB3	1.00	0.000	1.00	0.00
ARG53	HG2	1.00	0.000	1.00	0.00
ARG53	HG3	1.00	0.000	1.00	0.00
ARG53	HD2	1.00	0.000	1.00	0.00
ARG53	HD3	1.00	0.000	1.00	0.00
ARG53	H	1.00	0.000	1.00	0.00
GLN54	H	0.97	0.000	1.00	0.00

**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	0.000	1.00	0.00
ARG53	HB2	1.00	0.000	1.00	0.00
ARG53	HB3	1.00	0.000	1.00	0.00
ARG53	HG2	1.00	0.000	1.00	0.00
ARG53	HG3	1.00	0.000	1.00	0.00
ARG53	HD2	1.00	0.000	1.00	0.00
ARG53	HD3	1.00	0.000	1.00	0.00
ARG53	H	1.00	0.000	1.00	0.00
GLN54	H	0.96	0.000	1.00	0.00

**3.53.11 Detailed Probabilities of ARG53HD2:**

Overall probability: 1.000

Overall confidence: 0.700

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ARG53	1.00	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	0.00
ARG53	HB2	1.00	0.000	1.00	0.00
ARG53	HB3	1.00	0.000	1.00	0.00
ARG53	HG2	1.00	0.000	1.00	0.00
ARG53	HG3	1.00	0.000	1.00	0.00
ARG53	HD2	1.00	0.000	1.00	0.00
ARG53	HD3	1.00	0.000	1.00	0.00
ARG53	H	0.87	0.000	1.00	0.00

**3.53.12 Detailed Probabilities of ARG53HD3:**

Overall probability: 1.000

Overall confidence: 0.700

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ARG53	1.00	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	0.000	1.00	0.00
ARG53	HB2	1.00	0.000	1.00	0.00
ARG53	HB3	1.00	0.000	1.00	0.00
ARG53	HG2	1.00	0.000	1.00	0.00
ARG53	HG3	1.00	0.000	1.00	0.00
ARG53	HD2	1.00	0.000	1.00	0.00
ARG53	HD3	1.00	0.000	1.00	0.00
ARG53	H	0.86	0.000	1.00	0.00

**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	0.000	1.00	0.00
ALA52	HB1	1.00	0.000	1.00	0.00
ALA52	H	1.00	0.000	1.00	0.00
ARG53	HA	1.00	0.000	1.00	0.00
ARG53	HB2	1.00	0.000	1.00	0.00
ARG53	HB3	1.00	0.000	1.00	0.00
ARG53	HG2	1.00	0.000	1.00	0.00
ARG53	HG3	1.00	0.015	1.00	0.00
ARG53	H	1.00	0.000	1.00	0.00
ARG53	HD2	0.87	0.000	1.00	0.00
ARG53	HD3	0.86	0.000	1.00	0.00
GLN54	H	1.00	0.000	1.00	0.00
GLN54	HA	0.90	0.003	1.00	0.00

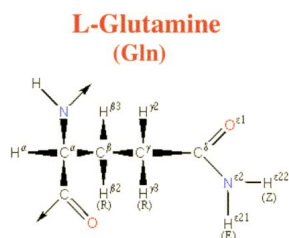


Figure 44: Image from the BMRB

Residue probability: 0.952

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	0.900	1.000
CB 3.54.2	28.314	29.436	2.799	0.900	1.000
CG 3.54.3	33.720	33.781	1.871	1.000	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	0.909	1.000
HB2 3.54.7	2.076	2.047	0.290	1.000	1.000
HB3 3.54.8	2.077	2.012	0.313	1.000	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	1.000	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: 0.900

Overall confidence: 1.000

### Inter- and intra-residue probability

Residue	Probability	Confidence
ARG53	0.50	1.00
GLN54	1.00	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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG53	HA	1.00	0.201	0.00	0.00
ARG53	H	0.90	0.003	1.00	0.00
GLN54	HA	1.00	0.000	1.00	0.00
GLN54	HB2	1.00	0.000	1.00	0.00
GLN54	HB3	1.00	0.000	1.00	0.00
GLN54	HG2	1.00	0.000	1.00	0.00
GLN54	HG3	1.00	0.000	1.00	0.00
GLN54	H	1.00	0.000	1.00	0.00
LEU55	HA	1.00	0.004	1.00	0.00
LEU55	H	1.00	0.000	1.00	0.00

**3.54.2 Detailed Probabilities of GLN54CB:**

Overall probability: 0.900

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
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	0.000	1.00	0.00
GLN54	HB2	1.00	0.000	1.00	0.00
GLN54	HB3	1.00	0.000	1.00	0.00
GLN54	HG2	1.00	0.000	1.00	0.00
GLN54	HG3	1.00	0.000	1.00	0.00
GLN54	H	1.00	0.000	1.00	0.00
GLN54	HE21	1.00	0.008	1.00	0.00
GLN54	HE22	1.00	0.543	0.00	0.00
LEU55	H	1.00	0.000	1.00	0.00
LEU55	HA	0.87	0.025	1.00	0.00

## 3.54.3 Detailed Probabilities of GLN54CG:

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	0.000	1.00	0.00
GLN54	HB2	1.00	0.000	1.00	0.00
GLN54	HB3	1.00	0.000	1.00	0.00
GLN54	HG2	1.00	0.000	1.00	0.00
GLN54	HG3	1.00	0.000	1.00	0.00
GLN54	H	1.00	0.000	1.00	0.00
GLN54	HE21	1.00	0.000	1.00	0.00
GLN54	HE22	1.00	0.000	1.00	0.00
LEU55	H	0.98	0.000	1.00	0.00

## 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	0.000	1.00	0.00
ARG53	HB2	1.00	0.000	1.00	0.00
ARG53	HB3	1.00	0.000	1.00	0.00
ARG53	HG2	0.97	0.000	1.00	0.00
ARG53	HG3	0.96	0.000	1.00	0.00
ARG53	H	1.00	0.000	1.00	0.00
GLN54	HA	1.00	0.000	1.00	0.00
GLN54	HB2	1.00	0.000	1.00	0.00
GLN54	HB3	1.00	0.000	1.00	0.00
GLN54	HG2	1.00	0.000	1.00	0.00
GLN54	HG3	1.00	0.000	1.00	0.00
GLN54	H	1.00	0.000	1.00	0.00
LEU55	H	1.00	0.000	1.00	0.00
LEU55	HA	0.94	0.025	1.00	0.00

**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	0.000	1.00	0.00
GLN54	HB3	1.00	0.000	1.00	0.00
GLN54	HG2	1.00	0.000	1.00	0.00
GLN54	HG3	1.00	0.000	1.00	0.00
GLN54	HE21	1.00	0.000	1.00	0.00
GLN54	HE22	1.00	0.000	1.00	0.00
GLN54	HA	0.94	0.000	1.00	0.00

**3.54.6 Detailed Probabilities of GLN54HA:**

Overall probability: 0.909

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ARG53	0.50	1.00
GLN54	1.00	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	0.201	0.00	0.00
ARG53	HB3	0.79	0.004	1.00	0.00
GLN54	HA	1.00	0.000	1.00	0.00
GLN54	HB2	1.00	0.000	1.00	0.00
GLN54	HB3	1.00	0.000	1.00	0.00
GLN54	HG2	1.00	0.000	1.00	0.00
GLN54	HG3	1.00	0.000	1.00	0.00
GLN54	H	1.00	0.000	1.00	0.00
GLN54	HE21	0.94	0.000	1.00	0.00
LEU55	HA	1.00	0.002	1.00	0.00
LEU55	H	1.00	0.000	1.00	0.00

## 3.54.7 Detailed Probabilities of GLN54HB2:

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
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	0.000	1.00	0.00
GLN54	HB2	1.00	0.000	1.00	0.00
GLN54	HB3	1.00	0.000	1.00	0.00
GLN54	HG2	1.00	0.000	1.00	0.00
GLN54	HG3	1.00	0.000	1.00	0.00
GLN54	H	1.00	0.000	1.00	0.00
GLN54	HE21	1.00	0.000	1.00	0.00
GLN54	HE22	1.00	0.000	1.00	0.00
LEU55	H	1.00	0.000	1.00	0.00

**3.54.8 Detailed Probabilities of GLN54HB3:**

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
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	0.000	1.00	0.00
GLN54	HB2	1.00	0.000	1.00	0.00
GLN54	HB3	1.00	0.000	1.00	0.00
GLN54	HG2	1.00	0.000	1.00	0.00
GLN54	HG3	1.00	0.000	1.00	0.00
GLN54	H	1.00	0.000	1.00	0.00
GLN54	HE21	1.00	0.000	1.00	0.00
GLN54	HE22	1.00	0.000	1.00	0.00
LEU55	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
GLN54	HB2	1.00	0.000	1.00	0.00
GLN54	HB3	1.00	0.000	1.00	0.00
GLN54	HG2	1.00	0.000	1.00	0.00
GLN54	HG3	1.00	0.000	1.00	0.00
GLN54	H	1.00	0.000	1.00	0.00
GLN54	HE21	1.00	0.000	1.00	0.00
GLN54	HE22	1.00	0.000	1.00	0.00
LEU55	H	0.98	0.000	1.00	0.00

**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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN54	HA	1.00	0.000	1.00	0.00
GLN54	HB2	1.00	0.000	1.00	0.00
GLN54	HB3	1.00	0.000	1.00	0.00
GLN54	HG2	1.00	0.000	1.00	0.00
GLN54	HG3	1.00	0.000	1.00	0.00
GLN54	H	1.00	0.000	1.00	0.00
GLN54	HE21	1.00	0.000	1.00	0.00
GLN54	HE22	1.00	0.000	1.00	0.00
LEU55	H	0.97	0.000	1.00	0.00

## 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	0.000	1.00	0.00
ARG53	HB2	1.00	0.000	1.00	0.00
ARG53	HB3	1.00	0.000	1.00	0.00
ARG53	HG2	0.97	0.000	1.00	0.00
ARG53	HG3	0.96	0.000	1.00	0.00
ARG53	H	1.00	0.000	1.00	0.00
ARG53	HD2	0.54	0.000	1.00	0.00
ARG53	HD3	0.58	0.000	1.00	0.00
GLN54	HA	1.00	0.000	1.00	0.00
GLN54	HB2	1.00	0.000	1.00	0.00
GLN54	HB3	1.00	0.000	1.00	0.00
GLN54	HG2	1.00	0.000	1.00	0.00
GLN54	HG3	1.00	0.000	1.00	0.00
GLN54	H	1.00	0.000	1.00	0.00
LEU55	H	1.00	0.000	1.00	0.00

## 3.54.12 Detailed Probabilities of GLN54HE21:

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	0.008	1.00	0.00
GLN54	HB3	1.00	0.008	1.00	0.00
GLN54	HG2	1.00	0.000	1.00	0.00
GLN54	HG3	1.00	0.000	1.00	0.00
GLN54	HE21	1.00	0.000	1.00	0.00
GLN54	HE22	1.00	0.000	1.00	0.00

## 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	0.543	0.00	0.00
GLN54	HB3	1.00	0.543	0.00	0.00
GLN54	HG2	1.00	0.000	1.00	0.00
GLN54	HG3	1.00	0.000	1.00	0.00
GLN54	HE21	1.00	0.000	1.00	0.00
GLN54	HE22	1.00	0.000	1.00	0.00

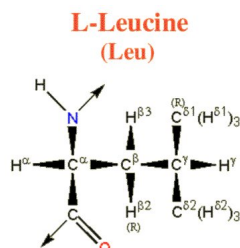
**3.55 LEU(55)**

Figure 45: Image from the BMRB

Residue probability: 0.986

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	0.900	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	1.000	1.000
CD1 3.55.4	26.807	24.837	3.657	1.000	1.000
CD2 3.55.5	24.046	24.201	3.117	1.000	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	0.923	1.000
HB2 3.55.8	1.870	1.601	0.373	1.000	1.000
HB3 3.55.9	0.914	1.508	0.398	1.000	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	1.000	1.000
HD2 3.55.12	0.717	0.727	0.421	1.000	1.000
H 3.55.13	8.106	8.237	0.647	1.000	1.000

**3.55.1 Detailed Probabilities of LEU55CA:**

Overall probability: 0.900

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLN54	1.00	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	0.002	1.00	0.00
LEU55	HA	1.00	0.000	1.00	0.00
LEU55	HB2	1.00	0.000	1.00	0.00
LEU55	HB3	1.00	0.000	1.00	0.00
LEU55	HG	1.00	0.000	1.00	0.00
LEU55	HD11	0.99	0.000	1.00	0.00
LEU55	HD21	0.99	0.000	1.00	0.00
LEU55	H	1.00	0.000	1.00	0.00
PHE56	HA	1.00	0.081	0.00	0.00
PHE56	H	1.00	0.000	1.00	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
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**

## 3.55 LEU(55)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU55	HA	1.00	0.000	1.00	0.00
LEU55	HB2	1.00	0.000	1.00	0.00
LEU55	HB3	1.00	0.000	1.00	0.00
LEU55	HG	1.00	0.000	1.00	0.00
LEU55	HD11	1.00	0.000	1.00	0.00
LEU55	HD21	1.00	0.000	1.00	0.00
LEU55	H	1.00	0.000	1.00	0.00
PHE56	H	1.00	0.000	1.00	0.00

## 3.55.3 Detailed Probabilities of LEU55CG:

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	0.000	1.00	0.00
LEU55	HB2	1.00	0.000	1.00	0.00
LEU55	HB3	1.00	0.000	1.00	0.00
LEU55	HG	1.00	0.000	1.00	0.00
LEU55	HD11	1.00	0.000	1.00	0.00
LEU55	HD21	1.00	0.000	1.00	0.00
LEU55	H	1.00	0.000	1.00	0.00
PHE56	H	0.98	0.000	1.00	0.00

## 3.55.4 Detailed Probabilities of LEU55CD1:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
LEU55	1.00	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	0.000	1.00	0.00
LEU55	HB2	1.00	0.000	1.00	0.00
LEU55	HB3	1.00	0.000	1.00	0.00
LEU55	HG	1.00	0.000	1.00	0.00
LEU55	HD11	1.00	0.000	1.00	0.00
LEU55	HD21	1.00	0.000	1.00	0.00
LEU55	H	0.86	0.000	1.00	0.00

**3.55.5 Detailed Probabilities of LEU55CD2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU55	1.00	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	0.000	1.00	0.00
LEU55	HB2	1.00	0.000	1.00	0.00
LEU55	HB3	1.00	0.000	1.00	0.00
LEU55	HG	1.00	0.000	1.00	0.00
LEU55	HD11	1.00	0.000	1.00	0.00
LEU55	HD21	1.00	0.000	1.00	0.00
LEU55	H	0.85	0.000	1.00	0.00

**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	0.000	1.00	0.00
GLN54	HB2	1.00	0.000	1.00	0.00
GLN54	HB3	1.00	0.000	1.00	0.00
GLN54	HG2	0.98	0.000	1.00	0.00
GLN54	HG3	0.97	0.000	1.00	0.00
GLN54	H	1.00	0.000	1.00	0.00
LEU55	HA	1.00	0.000	1.00	0.00
LEU55	HB2	1.00	0.000	1.00	0.00
LEU55	HB3	1.00	0.000	1.00	0.00
LEU55	HG	1.00	0.000	1.00	0.00
LEU55	H	1.00	0.000	1.00	0.00
LEU55	HD11	0.88	0.000	1.00	0.00
LEU55	HD21	0.87	0.000	1.00	0.00
PHE56	H	1.00	0.000	1.00	0.00
PHE56	HB2	0.58	0.002	1.00	0.00

**3.55.7 Detailed Probabilities of LEU55HA:**

Overall probability: 0.923

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLN54	1.00	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	0.004	1.00	0.00
GLN54	HB2	0.72	0.025	1.00	0.00
GLN54	HB3	0.87	0.025	1.00	0.00
GLN54	H	0.94	0.025	1.00	0.00
LEU55	HA	1.00	0.000	1.00	0.00
LEU55	HB2	1.00	0.000	1.00	0.00
LEU55	HB3	1.00	0.000	1.00	0.00
LEU55	HG	1.00	0.000	1.00	0.00
LEU55	HD11	0.99	0.000	1.00	0.00
LEU55	HD21	0.99	0.000	1.00	0.00
LEU55	H	1.00	0.000	1.00	0.00
PHE56	HA	1.00	0.081	0.00	0.00
PHE56	H	1.00	0.000	1.00	0.00

**3.55.8 Detailed Probabilities of LEU55HB2:**

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
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	0.000	1.00	0.00
LEU55	HB2	1.00	0.000	1.00	0.00
LEU55	HB3	1.00	0.000	1.00	0.00
LEU55	HG	1.00	0.000	1.00	0.00
LEU55	HD11	1.00	0.000	1.00	0.00
LEU55	HD21	1.00	0.000	1.00	0.00
LEU55	H	1.00	0.000	1.00	0.00
PHE56	H	1.00	0.000	1.00	0.00

**3.55.9 Detailed Probabilities of LEU55HB3:**

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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU55	HA	1.00	0.000	1.00	0.00
LEU55	HB2	1.00	0.000	1.00	0.00
LEU55	HB3	1.00	0.000	1.00	0.00
LEU55	HG	1.00	0.000	1.00	0.00
LEU55	HD11	1.00	0.000	1.00	0.00
LEU55	HD21	1.00	0.000	1.00	0.00
LEU55	H	1.00	0.000	1.00	0.00
PHE56	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
LEU55	HB2	1.00	0.000	1.00	0.00
LEU55	HB3	1.00	0.000	1.00	0.00
LEU55	HG	1.00	0.000	1.00	0.00
LEU55	HD11	1.00	0.000	1.00	0.00
LEU55	HD21	1.00	0.000	1.00	0.00
LEU55	H	1.00	0.000	1.00	0.00
PHE56	H	0.98	0.000	1.00	0.00

**3.55.11 Detailed Probabilities of LEU55HD11:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU55	1.00	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	0.000	1.00	0.00
LEU55	HB2	1.00	0.000	1.00	0.00
LEU55	HB3	1.00	0.000	1.00	0.00
LEU55	HG	1.00	0.000	1.00	0.00
LEU55	HD11	1.00	0.000	1.00	0.00
LEU55	HD21	1.00	0.000	1.00	0.00
LEU55	H	0.86	0.000	1.00	0.00

**3.55.12 Detailed Probabilities of LEU55HD21:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU55	1.00	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	0.000	1.00	0.00
LEU55	HB2	1.00	0.000	1.00	0.00
LEU55	HB3	1.00	0.000	1.00	0.00
LEU55	HG	1.00	0.000	1.00	0.00
LEU55	HD11	1.00	0.000	1.00	0.00
LEU55	HD21	1.00	0.000	1.00	0.00
LEU55	H	0.85	0.000	1.00	0.00

**3.55.13 Detailed Probabilities of LEU55H:**

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	0.000	1.00	0.00
GLN54	HB2	1.00	0.000	1.00	0.00
GLN54	HB3	1.00	0.000	1.00	0.00
GLN54	HG2	0.98	0.000	1.00	0.00
GLN54	HG3	0.97	0.000	1.00	0.00
GLN54	H	1.00	0.000	1.00	0.00
LEU55	HA	1.00	0.000	1.00	0.00
LEU55	HB2	1.00	0.000	1.00	0.00
LEU55	HB3	1.00	0.000	1.00	0.00
LEU55	HG	1.00	0.000	1.00	0.00
LEU55	H	1.00	0.000	1.00	0.00
LEU55	HD11	0.88	0.000	1.00	0.00
LEU55	HD21	0.87	0.000	1.00	0.00
PHE56	H	1.00	0.000	1.00	0.00

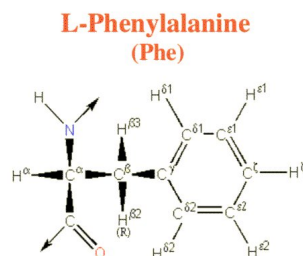


Figure 46: Image from the BMRB

**Residue probability:** 0.976  
**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	0.800	1.000
CB 3.56.2	38.913	40.078	3.616	1.000	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	1.000	1.000
CE2 3.56.6	131.004	130.633	2.839	1.000	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	1.000	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	1.000	1.000
HE2 3.56.15	7.002	7.043	0.400	1.000	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	1.000	1.000

**3.56.1 Detailed Probabilities of PHE56CA:**

**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	0.081	0.00	0.00
PHE56	HA	1.00	0.000	1.00	0.00
PHE56	HB2	1.00	0.000	1.00	0.00
PHE56	HB3	1.00	0.000	1.00	0.00
PHE56	HD1	1.00	0.006	1.00	0.00
PHE56	HD2	1.00	0.006	1.00	0.00
PHE56	H	1.00	0.000	1.00	0.00
PHE56	HE1	0.74	0.017	1.00	0.00
ARG57	HA	1.00	0.104	0.00	0.00
ARG57	H	1.00	0.000	1.00	0.00

**3.56.2 Detailed Probabilities of PHE56CB:**

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
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**

## 3.56 PHE(56)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE56	HA	1.00	0.000	1.00	0.00
PHE56	HB2	1.00	0.000	1.00	0.00
PHE56	HB3	1.00	0.000	1.00	0.00
PHE56	HD1	1.00	0.006	1.00	0.00
PHE56	HD2	1.00	0.006	1.00	0.00
PHE56	HE2	1.00	0.006	1.00	0.00
PHE56	H	1.00	0.000	1.00	0.00
PHE56	HE1	0.90	0.006	1.00	0.00
ARG57	H	1.00	0.000	1.00	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	0.000	1.00	0.00
PHE56	HB2	1.00	0.000	1.00	0.00
PHE56	HB3	1.00	0.000	1.00	0.00
PHE56	HD1	1.00	0.004	1.00	0.00
PHE56	HD2	1.00	0.004	1.00	0.00
PHE56	HE1	1.00	0.003	1.00	0.00
PHE56	HE2	1.00	0.003	1.00	0.00
PHE56	HZ	1.00	0.004	1.00	0.00
PHE56	H	1.00	0.000	1.00	0.00

## 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	0.000	1.00	0.00
PHE56	HB2	1.00	0.000	1.00	0.00
PHE56	HB3	1.00	0.000	1.00	0.00
PHE56	HD1	1.00	0.004	1.00	0.00
PHE56	HD2	1.00	0.004	1.00	0.00
PHE56	HE1	1.00	0.003	1.00	0.00
PHE56	HE2	1.00	0.003	1.00	0.00
PHE56	HZ	1.00	0.004	1.00	0.00
PHE56	H	0.99	0.000	1.00	0.00

**3.56.5 Detailed Probabilities of PHE56CE1:**

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
F56HE2	1.00
F56HZ	1.00
F56HE1	1.00

**NOESY contacts detailed probability**

## 3.56 PHE(56)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE56	HD1	1.00	0.004	1.00	0.00
PHE56	HD2	1.00	0.004	1.00	0.00
PHE56	HE1	1.00	0.003	1.00	0.00
PHE56	HE2	1.00	0.003	1.00	0.00
PHE56	HZ	1.00	0.004	1.00	0.00
PHE56	HA	0.74	0.009	1.00	0.00
PHE56	HB2	0.90	0.006	1.00	0.00
PHE56	HB3	0.89	0.019	1.00	0.00

**3.56.6 Detailed Probabilities of PHE56CE2:**

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
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	0.006	1.00	0.00
PHE56	HB3	1.00	0.019	1.00	0.00
PHE56	HD1	1.00	0.004	1.00	0.00
PHE56	HD2	1.00	0.004	1.00	0.00
PHE56	HE1	1.00	0.003	1.00	0.00
PHE56	HE2	1.00	0.003	1.00	0.00
PHE56	HZ	1.00	0.004	1.00	0.00

**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	0.004	1.00	0.00
PHE56	HD2	1.00	0.004	1.00	0.00
PHE56	HE1	1.00	0.003	1.00	0.00
PHE56	HE2	1.00	0.003	1.00	0.00
PHE56	HZ	1.00	0.004	1.00	0.00

**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**

## 3.56 PHE(56)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU55	HA	1.00	0.000	1.00	0.00
LEU55	HB2	1.00	0.000	1.00	0.00
LEU55	HB3	1.00	0.000	1.00	0.00
LEU55	HG	0.98	0.000	1.00	0.00
LEU55	H	1.00	0.000	1.00	0.00
LEU55	HD11	0.55	0.000	1.00	0.00
LEU55	HD21	0.61	0.000	1.00	0.00
PHE56	HA	1.00	0.000	1.00	0.00
PHE56	HB2	1.00	0.000	1.00	0.00
PHE56	HB3	1.00	0.000	1.00	0.00
PHE56	HD1	1.00	0.006	1.00	0.00
PHE56	HD2	0.99	0.006	1.00	0.00
PHE56	H	1.00	0.000	1.00	0.00
ARG57	H	1.00	0.000	1.00	0.00

## 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	0.081	0.00	0.00
PHE56	HA	1.00	0.000	1.00	0.00
PHE56	HB2	1.00	0.000	1.00	0.00
PHE56	HB3	1.00	0.000	1.00	0.00
PHE56	HD1	1.00	0.000	1.00	0.00
PHE56	HD2	1.00	0.000	1.00	0.00
PHE56	H	1.00	0.000	1.00	0.00
PHE56	HE1	0.74	0.009	1.00	0.00
ARG57	HA	1.00	0.104	0.00	0.00
ARG57	H	1.00	0.000	1.00	0.00

**3.56.10 Detailed Probabilities of PHE56HB2:**

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
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	0.000	1.00	0.00
PHE56	HB2	1.00	0.000	1.00	0.00
PHE56	HB3	1.00	0.000	1.00	0.00
PHE56	HD1	1.00	0.000	1.00	0.00
PHE56	HD2	1.00	0.000	1.00	0.00
PHE56	HE2	1.00	0.006	1.00	0.00
PHE56	H	1.00	0.000	1.00	0.00
PHE56	HE1	0.90	0.006	1.00	0.00
ARG57	H	1.00	0.000	1.00	0.00
ARG57	HA	0.64	0.011	1.00	0.00

**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	0.000	1.00	0.00
PHE56	HB2	1.00	0.000	1.00	0.00
PHE56	HB3	1.00	0.000	1.00	0.00
PHE56	HD1	1.00	0.000	1.00	0.00
PHE56	HD2	1.00	0.000	1.00	0.00
PHE56	HE2	1.00	0.019	1.00	0.00
PHE56	H	1.00	0.000	1.00	0.00
PHE56	HE1	0.89	0.019	1.00	0.00
ARG57	H	1.00	0.000	1.00	0.00

**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	0.006	1.00	0.00
PHE56	HB2	1.00	0.006	1.00	0.00
PHE56	HB3	1.00	0.006	1.00	0.00
PHE56	HD1	1.00	0.004	1.00	0.00
PHE56	HD2	1.00	0.004	1.00	0.00
PHE56	HE1	1.00	0.004	1.00	0.00
PHE56	HE2	1.00	0.004	1.00	0.00
PHE56	HZ	1.00	0.004	1.00	0.00
PHE56	H	1.00	0.006	1.00	0.00

**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	0.006	1.00	0.00
PHE56	HB2	1.00	0.006	1.00	0.00
PHE56	HB3	1.00	0.006	1.00	0.00
PHE56	HD1	1.00	0.004	1.00	0.00
PHE56	HD2	1.00	0.004	1.00	0.00
PHE56	HE1	1.00	0.004	1.00	0.00
PHE56	HE2	1.00	0.004	1.00	0.00
PHE56	HZ	1.00	0.004	1.00	0.00
PHE56	H	0.99	0.006	1.00	0.00

**3.56.14 Detailed Probabilities of PHE56HE1:**

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
F56HE2	1.00
F56HZ	1.00
F56HE1	1.00

**NOESY contacts detailed probability**

## 3.56 PHE(56)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE56	HD1	1.00	0.003	1.00	0.00
PHE56	HD2	1.00	0.003	1.00	0.00
PHE56	HE1	1.00	0.003	1.00	0.00
PHE56	HE2	1.00	0.003	1.00	0.00
PHE56	HZ	1.00	0.003	1.00	0.00
PHE56	HA	0.74	0.017	1.00	0.00
PHE56	HB2	0.90	0.006	1.00	0.00
PHE56	HB3	0.89	0.022	1.00	0.00

**3.56.15 Detailed Probabilities of PHE56HE2:**

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
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	0.006	1.00	0.00
PHE56	HB3	1.00	0.022	1.00	0.00
PHE56	HD1	1.00	0.003	1.00	0.00
PHE56	HD2	1.00	0.003	1.00	0.00
PHE56	HE1	1.00	0.003	1.00	0.00
PHE56	HE2	1.00	0.003	1.00	0.00
PHE56	HZ	1.00	0.003	1.00	0.00

**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	0.004	1.00	0.00
PHE56	HD2	1.00	0.004	1.00	0.00
PHE56	HE1	1.00	0.004	1.00	0.00
PHE56	HE2	1.00	0.004	1.00	0.00
PHE56	HZ	1.00	0.004	1.00	0.00

**3.56.17 Detailed Probabilities of PHE56H:**

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**

## 3.56 PHE(56)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU55	HA	1.00	0.000	1.00	0.00
LEU55	HB2	1.00	0.000	1.00	0.00
LEU55	HB3	1.00	0.000	1.00	0.00
LEU55	HG	0.98	0.000	1.00	0.00
LEU55	H	1.00	0.000	1.00	0.00
LEU55	HD11	0.55	0.000	1.00	0.00
LEU55	HD21	0.61	0.000	1.00	0.00
PHE56	HA	1.00	0.000	1.00	0.00
PHE56	HB2	1.00	0.000	1.00	0.00
PHE56	HB3	1.00	0.000	1.00	0.00
PHE56	HD1	1.00	0.000	1.00	0.00
PHE56	HD2	0.99	0.000	1.00	0.00
PHE56	H	1.00	0.000	1.00	0.00
ARG57	H	1.00	0.000	1.00	0.00

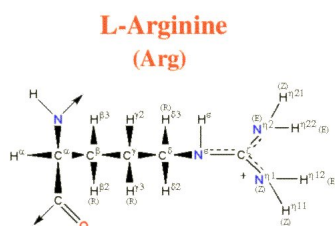


Figure 47: Image from the BMRB

Residue probability: 0.971  
 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	0.833	1.000
CB 3.57.2	29.511	30.892	2.424	1.000	0.889
CG 3.57.3	27.310	27.247	1.538	1.000	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	1.000	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	0.818	1.000
HB2 3.57.7	1.898	1.793	0.292	1.000	0.889
HB3 3.57.8	2.051	1.757	0.307	1.000	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	1.000	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	1.000	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: 0.833  
 Overall confidence: 1.000

#### Inter- and intra-residue probability

Residue	Probability	Confidence
PHE56	0.50	1.00
ARG57	1.00	1.00
ILE58	0.67	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	0.104	0.00	0.00
PHE56	HB2	0.64	0.011	1.00	0.00
ARG57	HA	1.00	0.000	1.00	0.00
ARG57	HB2	1.00	0.000	1.00	0.00
ARG57	HB3	1.00	0.000	1.00	0.00
ARG57	HG2	1.00	0.000	1.00	0.00
ARG57	HG3	1.00	0.000	1.00	0.00
ARG57	HD2	0.98	0.000	1.00	0.00
ARG57	H	1.00	0.000	1.00	0.00
ILE58	HA	1.00	0.352	0.00	0.00
ILE58	H	1.00	0.000	1.00	0.00
ILE58	HG12	0.51	0.007	1.00	0.00

**3.57.2 Detailed Probabilities of ARG57CB:**

Overall probability: 1.000

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ARG57	1.00	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	0.000	1.00	0.00
ARG57	HB2	1.00	0.000	1.00	0.00
ARG57	HB3	1.00	0.000	1.00	0.00
ARG57	HG2	1.00	0.000	1.00	0.00
ARG57	HG3	1.00	0.000	1.00	0.00
ARG57	HD2	1.00	0.000	1.00	0.00
ARG57	H	1.00	0.000	1.00	0.00
ILE58	H	1.00	0.000	1.00	0.00

**3.57.3 Detailed Probabilities of ARG57CG:**

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	0.000	1.00	0.00
ARG57	HB2	1.00	0.000	1.00	0.00
ARG57	HB3	1.00	0.000	1.00	0.00
ARG57	HG2	1.00	0.000	1.00	0.00
ARG57	HG3	1.00	0.000	1.00	0.00
ARG57	HD2	1.00	0.000	1.00	0.00
ARG57	H	1.00	0.000	1.00	0.00
ILE58	H	0.97	0.000	1.00	0.00

**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	0.000	1.00	0.00
ARG57	HB2	1.00	0.000	1.00	0.00
ARG57	HB3	1.00	0.000	1.00	0.00
ARG57	HG2	1.00	0.000	1.00	0.00
ARG57	HG3	1.00	0.000	1.00	0.00
ARG57	HD2	1.00	0.000	1.00	0.00
ARG57	H	0.86	0.000	1.00	0.00

**3.57.5 Detailed Probabilities of ARG57N:**

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
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	0.000	1.00	0.00
PHE56	HB2	1.00	0.000	1.00	0.00
PHE56	HB3	1.00	0.000	1.00	0.00
PHE56	H	1.00	0.000	1.00	0.00
ARG57	HA	1.00	0.000	1.00	0.00
ARG57	HB2	1.00	0.000	1.00	0.00
ARG57	HB3	1.00	0.000	1.00	0.00
ARG57	HG2	1.00	0.000	1.00	0.00
ARG57	HG3	1.00	0.000	1.00	0.00
ARG57	H	1.00	0.000	1.00	0.00
ARG57	HD2	0.87	0.000	1.00	0.00
ILE58	H	1.00	0.000	1.00	0.00
ILE58	HA	0.93	0.021	1.00	0.00
ILE58	HG13	0.55	0.020	1.00	0.00

**3.57.6 Detailed Probabilities of ARG57HA:**

Overall probability: 0.818

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE56	0.00	1.00
ARG57	1.00	1.00
ILE58	0.67	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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE56	HA	1.00	0.104	0.00	0.00
ARG57	HA	1.00	0.000	1.00	0.00
ARG57	HB2	1.00	0.000	1.00	0.00
ARG57	HB3	1.00	0.000	1.00	0.00
ARG57	HG2	1.00	0.000	1.00	0.00
ARG57	HG3	1.00	0.000	1.00	0.00
ARG57	HD2	0.98	0.000	1.00	0.00
ARG57	H	1.00	0.000	1.00	0.00
ILE58	HA	1.00	0.234	0.00	0.00
ILE58	H	1.00	0.000	1.00	0.00
ILE58	HG12	0.51	0.000	1.00	0.00

## 3.57.7 Detailed Probabilities of ARG57HB2:

Overall probability: 1.000

Overall confidence: 0.889

## Inter- and intra-residue probability

Residue	Probability	Confidence
ARG57	1.00	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	0.000	1.00	0.00
ARG57	HB2	1.00	0.000	1.00	0.00
ARG57	HB3	1.00	0.000	1.00	0.00
ARG57	HG2	1.00	0.000	1.00	0.00
ARG57	HG3	1.00	0.000	1.00	0.00
ARG57	HD2	1.00	0.000	1.00	0.00
ARG57	H	1.00	0.000	1.00	0.00
ILE58	H	1.00	0.000	1.00	0.00
ILE58	HA	0.67	0.013	1.00	0.00

**3.57.8 Detailed Probabilities of ARG57HB3:**

Overall probability: 1.000

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ARG57	1.00	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	0.000	1.00	0.00
ARG57	HB2	1.00	0.000	1.00	0.00
ARG57	HB3	1.00	0.000	1.00	0.00
ARG57	HG2	1.00	0.000	1.00	0.00
ARG57	HG3	1.00	0.000	1.00	0.00
ARG57	HD2	1.00	0.000	1.00	0.00
ARG57	H	1.00	0.000	1.00	0.00
ILE58	H	1.00	0.000	1.00	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	0.000	1.00	0.00
ARG57	HB2	1.00	0.000	1.00	0.00
ARG57	HB3	1.00	0.000	1.00	0.00
ARG57	HG2	1.00	0.000	1.00	0.00
ARG57	HG3	1.00	0.000	1.00	0.00
ARG57	HD2	1.00	0.000	1.00	0.00
ARG57	H	1.00	0.000	1.00	0.00
ILE58	H	0.97	0.000	1.00	0.00

**3.57.10 Detailed Probabilities of ARG57HG3:**

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
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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG57	HA	1.00	0.000	1.00	0.00
ARG57	HB2	1.00	0.000	1.00	0.00
ARG57	HB3	1.00	0.000	1.00	0.00
ARG57	HG2	1.00	0.000	1.00	0.00
ARG57	HG3	1.00	0.000	1.00	0.00
ARG57	HD2	1.00	0.000	1.00	0.00
ARG57	H	1.00	0.000	1.00	0.00
ILE58	H	0.96	0.000	1.00	0.00

## 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	0.000	1.00	0.00
ARG57	HB2	1.00	0.000	1.00	0.00
ARG57	HB3	1.00	0.000	1.00	0.00
ARG57	HG2	1.00	0.000	1.00	0.00
ARG57	HG3	1.00	0.000	1.00	0.00
ARG57	HD2	1.00	0.000	1.00	0.00
ARG57	H	0.86	0.000	1.00	0.00

## 3.57.12 Detailed Probabilities of ARG57H:

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
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	0.000	1.00	0.00
PHE56	HB2	1.00	0.000	1.00	0.00
PHE56	HB3	1.00	0.000	1.00	0.00
PHE56	H	1.00	0.000	1.00	0.00
PHE56	HD1	0.73	0.000	1.00	0.00
PHE56	HD2	0.68	0.000	1.00	0.00
ARG57	HA	1.00	0.000	1.00	0.00
ARG57	HB2	1.00	0.000	1.00	0.00
ARG57	HB3	1.00	0.000	1.00	0.00
ARG57	HG2	1.00	0.000	1.00	0.00
ARG57	HG3	1.00	0.000	1.00	0.00
ARG57	H	1.00	0.000	1.00	0.00
ARG57	HD2	0.87	0.000	1.00	0.00
ILE58	H	1.00	0.000	1.00	0.00

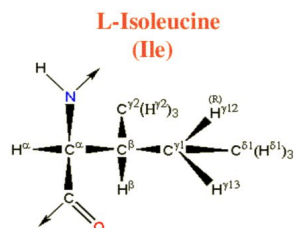


Figure 48: Image from the BMRB

Residue probability: 0.979  
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	0.909	1.000
CB 3.58.2	37.027	38.702	3.945	1.000	1.000
CG1 3.58.3	27.306	27.785	2.037	1.000	1.000
CG2 3.58.4	16.401	17.574	1.928	1.000	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	1.000	1.000
HA 3.58.7	3.859	4.185	1.403	0.818	1.000
HB 3.58.8	2.122	1.776	0.310	1.000	1.000
HG12 3.58.9	1.720	1.271	0.411	1.000	1.000
HG13 3.58.10	0.911	1.186	0.426	1.000	1.000
HG2 3.58.11	0.870	0.762	0.283	1.000	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: 0.909  
Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ARG57	0.50	1.00
ILE58	1.00	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	0.234	0.00	0.00
ARG57	HB2	0.67	0.013	1.00	0.00
ILE58	HA	1.00	0.000	1.00	0.00
ILE58	HB	1.00	0.000	1.00	0.00
ILE58	HG12	1.00	0.000	1.00	0.00
ILE58	HG13	1.00	0.000	1.00	0.00
ILE58	HG21	1.00	0.000	1.00	0.00
ILE58	HD11	0.97	0.000	1.00	0.00
ILE58	H	1.00	0.000	1.00	0.00
GLU59	HA	1.00	0.013	1.00	0.00
GLU59	H	1.00	0.000	1.00	0.00

**3.58.2 Detailed Probabilities of ILE58CB:**

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

**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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE58	HA	1.00	0.000	1.00	0.00
ILE58	HB	1.00	0.000	1.00	0.00
ILE58	HG12	1.00	0.000	1.00	0.00
ILE58	HG13	1.00	0.000	1.00	0.00
ILE58	HG21	1.00	0.000	1.00	0.00
ILE58	HD11	1.00	0.000	1.00	0.00
ILE58	H	1.00	0.000	1.00	0.00
GLU59	H	1.00	0.000	1.00	0.00

## 3.58.3 Detailed Probabilities of ILE58CG1:

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

## 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	0.000	1.00	0.00
ILE58	HB	1.00	0.000	1.00	0.00
ILE58	HG12	1.00	0.000	1.00	0.00
ILE58	HG13	1.00	0.000	1.00	0.00
ILE58	HG21	1.00	0.000	1.00	0.00
ILE58	HD11	1.00	0.000	1.00	0.00
ILE58	H	1.00	0.000	1.00	0.00
GLU59	H	0.98	0.000	1.00	0.00

## 3.58.4 Detailed Probabilities of ILE58CG2:

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

**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	0.000	1.00	0.00
ILE58	HB	1.00	0.000	1.00	0.00
ILE58	HG12	1.00	0.000	1.00	0.00
ILE58	HG13	1.00	0.000	1.00	0.00
ILE58	HG21	1.00	0.000	1.00	0.00
ILE58	HD11	0.99	0.000	1.00	0.00
ILE58	H	1.00	0.000	1.00	0.00
GLU59	H	0.98	0.000	1.00	0.00
GLU59	HA	0.67	0.010	1.00	0.00

**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	0.00
ILE58	HB	1.00	0.000	1.00	0.00
ILE58	HG12	1.00	0.000	1.00	0.00
ILE58	HG13	1.00	0.000	1.00	0.00
ILE58	HG21	0.99	0.000	1.00	0.00
ILE58	HD11	1.00	0.000	1.00	0.00
ILE58	H	0.94	0.000	1.00	0.00

**3.58.6 Detailed Probabilities of ILE58N:**

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	0.000	1.00	0.00
ARG57	HB2	1.00	0.000	1.00	0.00
ARG57	HB3	1.00	0.000	1.00	0.00
ARG57	HG2	0.97	0.000	1.00	0.00
ARG57	HG3	0.96	0.000	1.00	0.00
ARG57	H	1.00	0.000	1.00	0.00
ARG57	HD2	0.56	0.000	1.00	0.00
ILE58	HA	1.00	0.000	1.00	0.00
ILE58	HB	1.00	0.000	1.00	0.00
ILE58	HG12	1.00	0.000	1.00	0.00
ILE58	HG13	1.00	0.000	1.00	0.00
ILE58	HG21	1.00	0.000	1.00	0.00
ILE58	H	1.00	0.000	1.00	0.00
ILE58	HD11	0.94	0.000	1.00	0.00
GLU59	H	1.00	0.000	1.00	0.00
GLU59	HA	0.93	0.018	1.00	0.00
GLU59	HB2	0.55	0.003	1.00	0.00

**3.58.7 Detailed Probabilities of ILE58HA:**

Overall probability: 0.818

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ARG57	0.50	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	0.352	0.00	0.00
ARG57	H	0.93	0.021	1.00	0.00
ILE58	HA	1.00	0.000	1.00	0.00
ILE58	HB	1.00	0.000	1.00	0.00
ILE58	HG12	1.00	0.000	1.00	0.00
ILE58	HG13	1.00	0.000	1.00	0.00
ILE58	HG21	1.00	0.000	1.00	0.00
ILE58	HD11	0.97	0.000	1.00	0.00
ILE58	H	1.00	0.000	1.00	0.00
GLU59	HA	1.00	0.130	0.00	0.00
GLU59	H	1.00	0.000	1.00	0.00

**3.58.8 Detailed Probabilities of ILE58HB:**

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

**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	0.000	1.00	0.00
ILE58	HB	1.00	0.000	1.00	0.00
ILE58	HG12	1.00	0.000	1.00	0.00
ILE58	HG13	1.00	0.000	1.00	0.00
ILE58	HG21	1.00	0.000	1.00	0.00
ILE58	HD11	1.00	0.000	1.00	0.00
ILE58	H	1.00	0.000	1.00	0.00
GLU59	H	1.00	0.000	1.00	0.00

**3.58.9 Detailed Probabilities of ILE58HG12:**

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

**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	0.000	1.00	0.00
ILE58	HB	1.00	0.000	1.00	0.00
ILE58	HG12	1.00	0.000	1.00	0.00
ILE58	HG13	1.00	0.000	1.00	0.00
ILE58	HG21	1.00	0.000	1.00	0.00
ILE58	HD11	1.00	0.000	1.00	0.00
ILE58	H	1.00	0.000	1.00	0.00
GLU59	H	0.98	0.000	1.00	0.00

**3.58.10 Detailed Probabilities of ILE58HG13:**

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

**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	0.000	1.00	0.00
ILE58	HB	1.00	0.000	1.00	0.00
ILE58	HG12	1.00	0.000	1.00	0.00
ILE58	HG13	1.00	0.000	1.00	0.00
ILE58	HG21	1.00	0.000	1.00	0.00
ILE58	HD11	1.00	0.000	1.00	0.00
ILE58	H	1.00	0.000	1.00	0.00
GLU59	H	0.95	0.000	1.00	0.00

**3.58.11 Detailed Probabilities of ILE58HG21:**

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

**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	0.000	1.00	0.00
ILE58	HB	1.00	0.000	1.00	0.00
ILE58	HG12	1.00	0.000	1.00	0.00
ILE58	HG13	1.00	0.000	1.00	0.00
ILE58	HG21	1.00	0.000	1.00	0.00
ILE58	HD11	0.99	0.000	1.00	0.00
ILE58	H	1.00	0.000	1.00	0.00
GLU59	H	0.98	0.000	1.00	0.00

**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	0.000	1.00	0.00
ILE58	HB	1.00	0.000	1.00	0.00
ILE58	HG12	1.00	0.000	1.00	0.00
ILE58	HG13	1.00	0.000	1.00	0.00
ILE58	HG21	0.99	0.000	1.00	0.00
ILE58	HD11	1.00	0.000	1.00	0.00
ILE58	H	0.94	0.000	1.00	0.00

**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	0.000	1.00	0.00
ARG57	HB2	1.00	0.000	1.00	0.00
ARG57	HB3	1.00	0.000	1.00	0.00
ARG57	HG2	0.97	0.000	1.00	0.00
ARG57	HG3	0.96	0.000	1.00	0.00
ARG57	H	1.00	0.000	1.00	0.00
ARG57	HD2	0.56	0.000	1.00	0.00
ILE58	HA	1.00	0.000	1.00	0.00
ILE58	HB	1.00	0.000	1.00	0.00
ILE58	HG12	1.00	0.000	1.00	0.00
ILE58	HG13	1.00	0.000	1.00	0.00
ILE58	HG21	1.00	0.000	1.00	0.00
ILE58	H	1.00	0.000	1.00	0.00
ILE58	HD11	0.94	0.000	1.00	0.00
GLU59	H	1.00	0.000	1.00	0.00
GLU59	HA	0.93	0.002	1.00	0.00

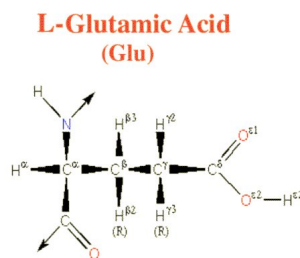
**3.59 GLU(59)**

Figure 49: Image from the BMRB

Residue probability: 0.982

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	0.818	1.000
CB 3.59.2	28.735	30.185	4.018	1.000	0.875
CG 3.59.3	36.010	36.085	1.533	1.000	0.875
N 3.59.4	129.678	120.574	4.837	1.000	1.000
HA 3.59.5	3.990	4.245	0.429	1.000	1.000
HB2 3.59.6	1.941	2.021	0.233	1.000	0.875
HB3 3.59.7	1.990	1.994	0.244	1.000	0.875
HG2 3.59.8	2.293	2.258	0.226	1.000	0.875
HG3 3.59.9	2.233	2.233	0.232	1.000	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: 0.818

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE58	0.50	1.00
GLU59	1.00	1.00
GLY60	0.67	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	0.130	0.00	0.00
ILE58	H	0.93	0.002	1.00	0.00
GLU59	HA	1.00	0.000	1.00	0.00
GLU59	HB2	1.00	0.000	1.00	0.00
GLU59	HB3	1.00	0.000	1.00	0.00
GLU59	HG2	1.00	0.000	1.00	0.00
GLU59	HG3	1.00	0.000	1.00	0.00
GLU59	H	1.00	0.000	1.00	0.00
GLY60	HA2	1.00	0.000	1.00	0.00
GLY60	HA3	1.00	0.230	0.00	0.00
GLY60	H	1.00	0.000	1.00	0.00

**3.59.2 Detailed Probabilities of GLU59CB:**

Overall probability: 1.000

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU59	1.00	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**

## 3.59 GLU(59)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU59	HA	1.00	0.000	1.00	0.00
GLU59	HB2	1.00	0.000	1.00	0.00
GLU59	HB3	1.00	0.000	1.00	0.00
GLU59	HG2	1.00	0.000	1.00	0.00
GLU59	HG3	1.00	0.000	1.00	0.00
GLU59	H	1.00	0.000	1.00	0.00
GLY60	H	1.00	0.000	1.00	0.00

## 3.59.3 Detailed Probabilities of GLU59CG:

Overall probability: 1.000

Overall confidence: 0.875

## Inter- and intra-residue probability

Residue	Probability	Confidence
GLU59	1.00	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	0.000	1.00	0.00
GLU59	HB2	1.00	0.000	1.00	0.00
GLU59	HB3	1.00	0.000	1.00	0.00
GLU59	HG2	1.00	0.000	1.00	0.00
GLU59	HG3	1.00	0.000	1.00	0.00
GLU59	H	1.00	0.000	1.00	0.00
GLY60	H	0.96	0.000	1.00	0.00

## 3.59.4 Detailed Probabilities of GLU59N:

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	0.000	1.00	0.00
ILE58	HB	1.00	0.000	1.00	0.00
ILE58	HG12	0.98	0.000	1.00	0.00
ILE58	HG13	0.95	0.000	1.00	0.00
ILE58	HG21	0.99	0.000	1.00	0.00
ILE58	H	1.00	0.000	1.00	0.00
GLU59	HA	1.00	0.000	1.00	0.00
GLU59	HB2	1.00	0.000	1.00	0.00
GLU59	HB3	1.00	0.000	1.00	0.00
GLU59	HG2	1.00	0.000	1.00	0.00
GLU59	HG3	1.00	0.000	1.00	0.00
GLU59	H	1.00	0.000	1.00	0.00
GLY60	H	1.00	0.000	1.00	0.00

**3.59.5 Detailed Probabilities of GLU59HA:**

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
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	0.013	1.00	0.00
ILE58	HG21	0.69	0.010	1.00	0.00
ILE58	H	0.93	0.018	1.00	0.00
GLU59	HA	1.00	0.000	1.00	0.00
GLU59	HB2	1.00	0.000	1.00	0.00
GLU59	HB3	1.00	0.000	1.00	0.00
GLU59	HG2	1.00	0.000	1.00	0.00
GLU59	HG3	1.00	0.000	1.00	0.00
GLU59	H	1.00	0.000	1.00	0.00
GLY60	HA2	1.00	0.002	1.00	0.00
GLY60	HA3	1.00	0.002	1.00	0.00
GLY60	H	1.00	0.000	1.00	0.00

**3.59.6 Detailed Probabilities of GLU59HB2:**

Overall probability: 1.000

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU59	1.00	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**

## 3.59 GLU(59)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU59	HA	1.00	0.000	1.00	0.00
GLU59	HB2	1.00	0.000	1.00	0.00
GLU59	HB3	1.00	0.000	1.00	0.00
GLU59	HG2	1.00	0.000	1.00	0.00
GLU59	HG3	1.00	0.000	1.00	0.00
GLU59	H	1.00	0.000	1.00	0.00
GLY60	H	1.00	0.000	1.00	0.00

## 3.59.7 Detailed Probabilities of GLU59HB3:

Overall probability: 1.000

Overall confidence: 0.875

## Inter- and intra-residue probability

Residue	Probability	Confidence
GLU59	1.00	0.86
GLY60	1.00	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	0.000	1.00	0.00
GLU59	HB2	1.00	0.000	1.00	0.00
GLU59	HB3	1.00	0.000	1.00	0.00
GLU59	HG2	1.00	0.000	1.00	0.00
GLU59	HG3	1.00	0.000	1.00	0.00
GLU59	H	1.00	0.000	1.00	0.00
GLY60	H	1.00	0.000	1.00	0.00

## 3.59.8 Detailed Probabilities of GLU59HG2:

Overall probability: 1.000

Overall confidence: 0.875

## Inter- and intra-residue probability

Residue	Probability	Confidence
GLU59	1.00	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	0.000	1.00	0.00
GLU59	HB2	1.00	0.000	1.00	0.00
GLU59	HB3	1.00	0.000	1.00	0.00
GLU59	HG2	1.00	0.000	1.00	0.00
GLU59	HG3	1.00	0.000	1.00	0.00
GLU59	H	1.00	0.000	1.00	0.00
GLY60	H	0.96	0.000	1.00	0.00

**3.59.9 Detailed Probabilities of GLU59HG3:**

Overall probability: 1.000

Overall confidence: 0.857

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU59	1.00	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	0.000	1.00	0.00
GLU59	HB2	1.00	0.000	1.00	0.00
GLU59	HB3	1.00	0.000	1.00	0.00
GLU59	HG2	1.00	0.000	1.00	0.00
GLU59	HG3	1.00	0.000	1.00	0.00
GLU59	H	1.00	0.000	1.00	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	0.000	1.00	0.00
ILE58	HB	1.00	0.000	1.00	0.00
ILE58	HG12	0.98	0.000	1.00	0.00
ILE58	HG13	0.95	0.000	1.00	0.00
ILE58	HG21	0.99	0.000	1.00	0.00
ILE58	H	1.00	0.000	1.00	0.00
GLU59	HA	1.00	0.000	1.00	0.00
GLU59	HB2	1.00	0.000	1.00	0.00
GLU59	HB3	1.00	0.000	1.00	0.00
GLU59	HG2	1.00	0.000	1.00	0.00
GLU59	HG3	1.00	0.000	1.00	0.00
GLU59	H	1.00	0.000	1.00	0.00
GLY60	H	1.00	0.000	1.00	0.00

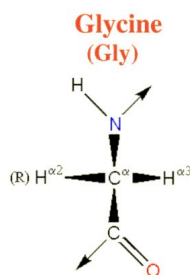
**3.60 GLY(60)**

Figure 50: Image from the BMRB

Residue probability: 0.867

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	0.833	1.000
N 3.60.2	112.584	109.752	5.331	1.000	1.000
HA2 3.60.3	3.528	3.967	0.380	0.833	1.000
HA3 3.60.4	4.423	3.897	0.390	0.667	1.000
H 3.60.5	8.682	8.343	0.939	1.000	1.000

**3.60.1 Detailed Probabilities of GLY60CA:**

Overall probability: 0.833

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU59	1.00	1.00
GLY60	1.00	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	0.002	1.00	0.00
GLY60	HA2	1.00	0.000	1.00	0.00
GLY60	HA3	1.00	0.000	1.00	0.00
GLY60	H	1.00	0.000	1.00	0.00
VAL61	HA	1.00	0.076	0.00	0.00
VAL61	H	1.00	0.000	1.00	0.00

**3.60.2 Detailed Probabilities of GLY60N:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU59	1.00	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	0.000	1.00	0.00
GLU59	HB2	1.00	0.000	1.00	0.00
GLU59	HB3	1.00	0.000	1.00	0.00
GLU59	HG2	0.96	0.000	1.00	0.00
GLU59	H	1.00	0.000	1.00	0.00
GLU59	HG3	0.93	0.000	1.00	0.00
GLY60	HA2	1.00	0.000	1.00	0.00
GLY60	HA3	1.00	0.000	1.00	0.00
GLY60	H	1.00	0.000	1.00	0.00
VAL61	H	1.00	0.000	1.00	0.00
VAL61	HB	0.52	0.002	1.00	0.00

**3.60.3 Detailed Probabilities of GLY60HA2:**

Overall probability: 0.833

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU59	1.00	1.00
GLY60	1.00	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	0.000	1.00	0.00
GLY60	HA2	1.00	0.000	1.00	0.00
GLY60	HA3	1.00	0.000	1.00	0.00
GLY60	H	1.00	0.000	1.00	0.00
VAL61	HA	1.00	0.076	0.00	0.00
VAL61	H	1.00	0.000	1.00	0.00

**3.60.4 Detailed Probabilities of GLY60HA3:**

Overall probability: 0.667

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU59	0.00	1.00
GLY60	1.00	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	0.230	0.00	0.00
GLY60	HA2	1.00	0.000	1.00	0.00
GLY60	HA3	1.00	0.000	1.00	0.00
GLY60	H	1.00	0.000	1.00	0.00
VAL61	HA	1.00	0.088	0.00	0.00
VAL61	H	1.00	0.000	1.00	0.00

**3.60.5 Detailed Probabilities of GLY60H:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU59	1.00	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	0.000	1.00	0.00
GLU59	HB2	1.00	0.000	1.00	0.00
GLU59	HB3	1.00	0.000	1.00	0.00
GLU59	HG2	0.96	0.000	1.00	0.00
GLU59	H	1.00	0.000	1.00	0.00
GLU59	HG3	0.93	0.000	1.00	0.00
GLY60	HA2	1.00	0.000	1.00	0.00
GLY60	HA3	1.00	0.000	1.00	0.00
GLY60	H	1.00	0.000	1.00	0.00
VAL61	H	1.00	0.000	1.00	0.00
VAL61	HB	0.52	0.003	1.00	0.00

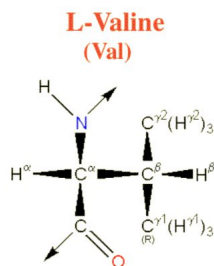


Figure 51: Image from the BMRB

**Residue probability:** 0.947  
**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	0.800	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	1.000	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	0.667	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	1.000	1.000
HG2 3.61.9	0.760	0.803	0.504	1.000	1.000
H 3.61.10	7.737	8.311	0.669	1.000	1.000

**3.61.1 Detailed Probabilities of VAL61CA:**

**Overall probability:** 0.800  
**Overall confidence:** 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLY60	0.00	1.00
VAL61	1.00	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	0.076	0.00	0.00
GLY60	HA3	1.00	0.088	0.00	0.00
VAL61	HA	1.00	0.000	1.00	0.00
VAL61	HB	1.00	0.000	1.00	0.00
VAL61	HG11	1.00	0.000	1.00	0.00
VAL61	HG21	1.00	0.000	1.00	0.00
VAL61	H	1.00	0.000	1.00	0.00
LYS62	HA	1.00	0.003	1.00	0.00
LYS62	H	1.00	0.000	1.00	0.00
LYS62	HB2	0.52	0.005	1.00	0.00

**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	0.000	1.00	0.00
VAL61	HB	1.00	0.000	1.00	0.00
VAL61	HG11	1.00	0.000	1.00	0.00
VAL61	HG21	1.00	0.000	1.00	0.00
VAL61	H	1.00	0.000	1.00	0.00
LYS62	H	1.00	0.000	1.00	0.00

**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	0.00
VAL61	HB	1.00	0.000	1.00	0.00
VAL61	HG11	1.00	0.000	1.00	0.00
VAL61	HG21	1.00	0.000	1.00	0.00
VAL61	H	1.00	0.000	1.00	0.00
LYS62	H	0.98	0.000	1.00	0.00
LYS62	HA	0.56	0.003	1.00	0.00

**3.61.4 Detailed Probabilities of VAL61CG2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL61	1.00	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	0.00
VAL61	HB	1.00	0.000	1.00	0.00
VAL61	HG11	1.00	0.000	1.00	0.00
VAL61	HG21	1.00	0.000	1.00	0.00
VAL61	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
GLY60	HA3	1.00	0.000	1.00	0.00
GLY60	H	1.00	0.000	1.00	0.00
VAL61	HA	1.00	0.000	1.00	0.00
VAL61	HB	1.00	0.000	1.00	0.00
VAL61	HG11	1.00	0.000	1.00	0.00
VAL61	HG21	1.00	0.000	1.00	0.00
VAL61	H	1.00	0.000	1.00	0.00
LYS62	H	1.00	0.000	1.00	0.00

**3.61.6 Detailed Probabilities of VAL61HA:**

Overall probability: 0.667

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLY60	0.00	1.00
VAL61	1.00	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	0.076	0.00	0.00
GLY60	HA3	1.00	0.076	0.00	0.00
VAL61	HA	1.00	0.000	1.00	0.00
VAL61	HB	1.00	0.000	1.00	0.00
VAL61	HG11	1.00	0.000	1.00	0.00
VAL61	HG21	1.00	0.000	1.00	0.00
VAL61	H	1.00	0.000	1.00	0.00
LYS62	HA	1.00	0.186	0.00	0.00
LYS62	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
VAL61	HB	1.00	0.000	1.00	0.00
VAL61	HG11	1.00	0.000	1.00	0.00
VAL61	HG21	1.00	0.000	1.00	0.00
VAL61	H	1.00	0.000	1.00	0.00
LYS62	H	1.00	0.000	1.00	0.00

**3.61.8 Detailed Probabilities of VAL61HG11:**

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	0.00
VAL61	HB	1.00	0.000	1.00	0.00
VAL61	HG11	1.00	0.000	1.00	0.00
VAL61	HG21	1.00	0.000	1.00	0.00
VAL61	H	1.00	0.000	1.00	0.00
LYS62	H	0.98	0.000	1.00	0.00

**3.61.9 Detailed Probabilities of VAL61HG21:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL61	1.00	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**

## 3.61 VAL(61)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL61	HA	1.00	0.000	1.00	0.00
VAL61	HB	1.00	0.000	1.00	0.00
VAL61	HG11	1.00	0.000	1.00	0.00
VAL61	HG21	1.00	0.000	1.00	0.00
VAL61	H	1.00	0.000	1.00	0.00

## 3.61.10 Detailed Probabilities of VAL61H:

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	0.000	1.00	0.00
GLY60	HA3	1.00	0.000	1.00	0.00
GLY60	H	1.00	0.000	1.00	0.00
VAL61	HA	1.00	0.000	1.00	0.00
VAL61	HB	1.00	0.000	1.00	0.00
VAL61	HG11	1.00	0.000	1.00	0.00
VAL61	HG21	1.00	0.000	1.00	0.00
VAL61	H	1.00	0.000	1.00	0.00
LYS62	H	1.00	0.000	1.00	0.00
LYS62	HA	0.91	0.024	1.00	0.00

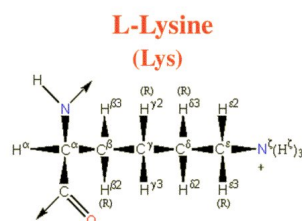


Figure 52: Image from the BMRB

Residue probability: 0.986  
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	0.854	1.000
CB 3.62.2	35.500	32.981	3.186	1.000	1.000
CG 3.62.3	24.553	24.941	1.956	1.000	0.917
CD 3.62.4	29.505	29.020	2.193	1.000	0.900
CE 3.62.5	41.780	41.893	1.492	1.000	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	0.929	1.000
HB2 3.62.8	1.426	1.774	0.365	1.000	1.000
HB3 3.62.9	1.345	1.742	0.385	1.000	1.000
HG2 3.62.10	1.556	1.358	0.344	1.000	0.917
HG3 3.62.11	1.416	1.343	0.357	1.000	0.917
HD2 3.62.12	1.603	1.614	0.957	1.000	0.900
HD3 3.62.13	1.740	1.595	0.387	1.000	0.900
HE2 3.62.14	3.058	2.907	0.230	1.000	0.889
HE3 3.62.15	3.060	2.901	0.241	1.000	0.889
H 3.62.16	9.311	8.185	0.605	1.000	1.000
HZ	NA	—	—	0.000	0.000

**3.62.1 Detailed Probabilities of LYS62CA:**

Overall probability: 0.854  
Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL61	0.60	1.00
LYS62	1.00	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	0.186	0.00	0.00
VAL61	HB	0.81	0.034	0.81	0.00
VAL61	H	0.91	0.024	1.00	0.00
LYS62	HA	1.00	0.000	1.00	0.00
LYS62	HB2	1.00	0.000	1.00	0.00
LYS62	HB3	1.00	0.000	1.00	0.00
LYS62	HG2	1.00	0.000	1.00	0.00
LYS62	HG3	1.00	0.000	1.00	0.00
LYS62	HD2	0.98	0.000	1.00	0.00
LYS62	HD3	0.98	0.000	1.00	0.00
LYS62	H	1.00	0.000	1.00	0.00
LYS62	HE2	0.77	0.000	1.00	0.00
LYS62	HE3	0.76	0.000	1.00	0.00
SER63	HA	1.00	0.472	0.00	0.00
SER63	H	1.00	0.000	1.00	0.00

**3.62.2 Detailed Probabilities of LYS62CB:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS62	1.00	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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS62	HA	1.00	0.000	1.00	0.00
LYS62	HB2	1.00	0.000	1.00	0.00
LYS62	HB3	1.00	0.000	1.00	0.00
LYS62	HG2	1.00	0.000	1.00	0.00
LYS62	HG3	1.00	0.000	1.00	0.00
LYS62	HD2	1.00	0.000	1.00	0.00
LYS62	HD3	1.00	0.000	1.00	0.00
LYS62	HE2	0.98	0.000	1.00	0.00
LYS62	HE3	0.99	0.000	1.00	0.00
LYS62	H	1.00	0.000	1.00	0.00
SER63	H	1.00	0.000	1.00	0.00

**3.62.3 Detailed Probabilities of LYS62CG:**

Overall probability: 1.000

Overall confidence: 0.917

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS62	1.00	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	0.000	1.00	0.00
LYS62	HB2	1.00	0.000	1.00	0.00
LYS62	HB3	1.00	0.000	1.00	0.00
LYS62	HG2	1.00	0.000	1.00	0.00
LYS62	HG3	1.00	0.000	1.00	0.00
LYS62	HD2	1.00	0.000	1.00	0.00
LYS62	HD3	1.00	0.000	1.00	0.00
LYS62	HE2	1.00	0.000	1.00	0.00
LYS62	HE3	1.00	0.000	1.00	0.00
LYS62	H	1.00	0.000	1.00	0.00
SER63	H	0.97	0.000	1.00	0.00

**3.62.4 Detailed Probabilities of LYS62CD:**

Overall probability: 1.000

Overall confidence: 0.900

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS62	1.00	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	0.000	1.00	0.00
LYS62	HB2	1.00	0.000	1.00	0.00
LYS62	HB3	1.00	0.000	1.00	0.00
LYS62	HG2	1.00	0.000	1.00	0.00
LYS62	HG3	1.00	0.000	1.00	0.00
LYS62	HD2	1.00	0.000	1.00	0.00
LYS62	HD3	1.00	0.000	1.00	0.00
LYS62	HE2	1.00	0.000	1.00	0.00
LYS62	HE3	1.00	0.000	1.00	0.00
LYS62	H	0.88	0.000	1.00	0.00

**3.62.5 Detailed Probabilities of LYS62CE:**

Overall probability: 1.000

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS62	1.00	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	0.000	1.00	0.00
LYS62	HB3	0.99	0.000	1.00	0.00
LYS62	HG2	1.00	0.000	1.00	0.00
LYS62	HG3	1.00	0.000	1.00	0.00
LYS62	HD2	1.00	0.000	1.00	0.00
LYS62	HD3	1.00	0.000	1.00	0.00
LYS62	HE2	1.00	0.000	1.00	0.00
LYS62	HE3	1.00	0.000	1.00	0.00
LYS62	HA	0.77	0.000	1.00	0.00

**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	0.000	1.00	0.00
VAL61	HB	1.00	0.000	1.00	0.00
VAL61	HG11	0.98	0.000	1.00	0.00
VAL61	HG21	0.95	0.000	1.00	0.00
VAL61	H	1.00	0.000	1.00	0.00
LYS62	HA	1.00	0.000	1.00	0.00
LYS62	HB2	1.00	0.000	1.00	0.00
LYS62	HB3	1.00	0.000	1.00	0.00
LYS62	HG2	1.00	0.000	1.00	0.00
LYS62	HG3	1.00	0.000	1.00	0.00
LYS62	H	1.00	0.000	1.00	0.00
LYS62	HD2	0.88	0.000	1.00	0.00
LYS62	HD3	0.87	0.000	1.00	0.00
SER63	H	1.00	0.000	1.00	0.00

**3.62.7 Detailed Probabilities of LYS62HA:**

Overall probability: 0.929

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL61	1.00	1.00
LYS62	1.00	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	0.003	1.00	0.00
VAL61	HG11	0.59	0.003	1.00	0.00
LYS62	HA	1.00	0.000	1.00	0.00
LYS62	HB2	1.00	0.000	1.00	0.00
LYS62	HB3	1.00	0.000	1.00	0.00
LYS62	HG2	1.00	0.000	1.00	0.00
LYS62	HG3	1.00	0.000	1.00	0.00
LYS62	HD2	0.98	0.000	1.00	0.00
LYS62	HD3	0.98	0.000	1.00	0.00
LYS62	H	1.00	0.000	1.00	0.00
LYS62	HE2	0.77	0.000	1.00	0.00
LYS62	HE3	0.76	0.000	1.00	0.00
SER63	HA	1.00	0.429	0.00	0.00
SER63	H	1.00	0.000	1.00	0.00

**3.62.8 Detailed Probabilities of LYS62HB2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS62	1.00	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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS62	HA	1.00	0.000	1.00	0.00
LYS62	HB2	1.00	0.000	1.00	0.00
LYS62	HB3	1.00	0.000	1.00	0.00
LYS62	HG2	1.00	0.000	1.00	0.00
LYS62	HG3	1.00	0.000	1.00	0.00
LYS62	HD2	1.00	0.000	1.00	0.00
LYS62	HD3	1.00	0.000	1.00	0.00
LYS62	HE2	0.98	0.000	1.00	0.00
LYS62	HE3	0.99	0.000	1.00	0.00
LYS62	H	1.00	0.000	1.00	0.00
SER63	H	1.00	0.000	1.00	0.00

**3.62.9 Detailed Probabilities of LYS62HB3:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS62	1.00	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	0.000	1.00	0.00
LYS62	HB2	1.00	0.000	1.00	0.00
LYS62	HB3	1.00	0.000	1.00	0.00
LYS62	HG2	1.00	0.000	1.00	0.00
LYS62	HG3	1.00	0.000	1.00	0.00
LYS62	HD2	1.00	0.000	1.00	0.00
LYS62	HD3	1.00	0.000	1.00	0.00
LYS62	HE2	0.99	0.000	1.00	0.00
LYS62	HE3	0.99	0.000	1.00	0.00
LYS62	H	1.00	0.000	1.00	0.00
SER63	H	1.00	0.000	1.00	0.00

**3.62.10 Detailed Probabilities of LYS62HG2:**

Overall probability: 1.000

Overall confidence: 0.917

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS62	1.00	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	0.000	1.00	0.00
LYS62	HB2	1.00	0.000	1.00	0.00
LYS62	HB3	1.00	0.000	1.00	0.00
LYS62	HG2	1.00	0.000	1.00	0.00
LYS62	HG3	1.00	0.000	1.00	0.00
LYS62	HD2	1.00	0.000	1.00	0.00
LYS62	HD3	1.00	0.000	1.00	0.00
LYS62	HE2	1.00	0.000	1.00	0.00
LYS62	HE3	1.00	0.000	1.00	0.00
LYS62	H	1.00	0.000	1.00	0.00
SER63	H	0.97	0.000	1.00	0.00

**3.62.11 Detailed Probabilities of LYS62HG3:**

Overall probability: 1.000

Overall confidence: 0.917

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS62	1.00	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	0.000	1.00	0.00
LYS62	HB2	1.00	0.000	1.00	0.00
LYS62	HB3	1.00	0.000	1.00	0.00
LYS62	HG2	1.00	0.000	1.00	0.00
LYS62	HG3	1.00	0.000	1.00	0.00
LYS62	HD2	1.00	0.000	1.00	0.00
LYS62	HD3	1.00	0.000	1.00	0.00
LYS62	HE2	1.00	0.000	1.00	0.00
LYS62	HE3	1.00	0.000	1.00	0.00
LYS62	H	1.00	0.000	1.00	0.00
SER63	H	0.96	0.000	1.00	0.00

**3.62.12 Detailed Probabilities of LYS62HD2:**

Overall probability: 1.000

Overall confidence: 0.900

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS62	1.00	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	0.000	1.00	0.00
LYS62	HB2	1.00	0.000	1.00	0.00
LYS62	HB3	1.00	0.000	1.00	0.00
LYS62	HG2	1.00	0.000	1.00	0.00
LYS62	HG3	1.00	0.000	1.00	0.00
LYS62	HD2	1.00	0.000	1.00	0.00
LYS62	HD3	1.00	0.000	1.00	0.00
LYS62	HE2	1.00	0.000	1.00	0.00
LYS62	HE3	1.00	0.000	1.00	0.00
LYS62	H	0.88	0.000	1.00	0.00

**3.62.13 Detailed Probabilities of LYS62HD3:**

Overall probability: 1.000

Overall confidence: 0.900

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS62	1.00	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	0.000	1.00	0.00
LYS62	HB2	1.00	0.000	1.00	0.00
LYS62	HB3	1.00	0.000	1.00	0.00
LYS62	HG2	1.00	0.000	1.00	0.00
LYS62	HG3	1.00	0.000	1.00	0.00
LYS62	HD2	1.00	0.000	1.00	0.00
LYS62	HD3	1.00	0.000	1.00	0.00
LYS62	HE2	1.00	0.000	1.00	0.00
LYS62	HE3	1.00	0.000	1.00	0.00
LYS62	H	0.87	0.000	1.00	0.00

**3.62.14 Detailed Probabilities of LYS62HE2:**

Overall probability: 1.000

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS62	1.00	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	0.000	1.00	0.00
LYS62	HB3	0.99	0.000	1.00	0.00
LYS62	HG2	1.00	0.000	1.00	0.00
LYS62	HG3	1.00	0.000	1.00	0.00
LYS62	HD2	1.00	0.000	1.00	0.00
LYS62	HD3	1.00	0.000	1.00	0.00
LYS62	HE2	1.00	0.000	1.00	0.00
LYS62	HE3	1.00	0.000	1.00	0.00
LYS62	HA	0.77	0.000	1.00	0.00

**3.62.15 Detailed Probabilities of LYS62HE3:**

Overall probability: 1.000

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS62	1.00	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	0.000	1.00	0.00
LYS62	HB3	0.99	0.000	1.00	0.00
LYS62	HG2	1.00	0.000	1.00	0.00
LYS62	HG3	1.00	0.000	1.00	0.00
LYS62	HD2	1.00	0.000	1.00	0.00
LYS62	HD3	1.00	0.000	1.00	0.00
LYS62	HE2	1.00	0.000	1.00	0.00
LYS62	HE3	1.00	0.000	1.00	0.00
LYS62	HA	0.76	0.000	1.00	0.00

**3.62.16 Detailed Probabilities of LYS62H:**

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**

## 3.62 LYS(62)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL61	HA	1.00	0.000	1.00	0.00
VAL61	HB	1.00	0.000	1.00	0.00
VAL61	HG11	0.98	0.000	1.00	0.00
VAL61	HG21	0.95	0.000	1.00	0.00
VAL61	H	1.00	0.000	1.00	0.00
LYS62	HA	1.00	0.000	1.00	0.00
LYS62	HB2	1.00	0.000	1.00	0.00
LYS62	HB3	1.00	0.000	1.00	0.00
LYS62	HG2	1.00	0.000	1.00	0.00
LYS62	HG3	1.00	0.000	1.00	0.00
LYS62	H	1.00	0.000	1.00	0.00
LYS62	HD2	0.88	0.000	1.00	0.00
LYS62	HD3	0.87	0.000	1.00	0.00
SER63	H	1.00	0.000	1.00	0.00

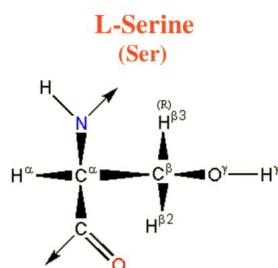


Figure 53: Image from the BMRB

**Residue probability:** 0.923  
**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	0.714	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	1.000	0.917
HA 3.63.4	4.986	4.486	0.430	0.750	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	1.000	0.833
H 3.63.7	7.713	8.292	0.600	1.000	0.917
HG	NA	—	—	0.000	0.000

**3.63.1 Detailed Probabilities of SER63CA:**

**Overall probability:** 0.714  
**Overall confidence:** 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS62	0.00	1.00
SER63	1.00	0.80
VAL64	0.50	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	0.429	0.00	0.00
SER63	HA	1.00	0.000	1.00	0.00
SER63	HB2	1.00	0.000	1.00	0.00
SER63	HB3	1.00	0.000	1.00	0.00
SER63	H	1.00	0.000	1.00	0.00
VAL64	HA	1.00	0.226	0.00	0.00
VAL64	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
SER63	HB2	1.00	0.000	1.00	0.00
SER63	HB3	1.00	0.000	1.00	0.00
SER63	H	1.00	0.000	1.00	0.00
VAL64	H	1.00	0.000	1.00	0.00

**3.63.3 Detailed Probabilities of SER63N:**

Overall probability: 1.000

Overall confidence: 0.917

**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
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	0.000	1.00	0.00
LYS62	HB2	1.00	0.000	1.00	0.00
LYS62	HB3	1.00	0.000	1.00	0.00
LYS62	HG2	0.97	0.000	1.00	0.00
LYS62	HG3	0.96	0.000	1.00	0.00
LYS62	H	1.00	0.000	1.00	0.00
SER63	HA	1.00	0.000	1.00	0.00
SER63	HB2	1.00	0.000	1.00	0.00
SER63	HB3	1.00	0.000	1.00	0.00
SER63	H	1.00	0.000	1.00	0.00
VAL64	H	1.00	0.000	1.00	0.00

**3.63.4 Detailed Probabilities of SER63HA:**

Overall probability: 0.750

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS62	0.00	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	0.472	0.00	0.00
SER63	HA	1.00	0.000	1.00	0.00
SER63	HB2	1.00	0.000	1.00	0.00
SER63	HB3	1.00	0.000	1.00	0.00
SER63	H	1.00	0.000	1.00	0.00
VAL64	HA	1.00	0.226	0.00	0.00
VAL64	H	1.00	0.000	1.00	0.00
VAL64	HB	0.52	0.004	1.00	0.00

**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	0.000	1.00	0.00
SER63	HB2	1.00	0.000	1.00	0.00
SER63	HB3	1.00	0.000	1.00	0.00
SER63	H	1.00	0.000	1.00	0.00
VAL64	H	1.00	0.000	1.00	0.00

**3.63.6 Detailed Probabilities of SER63HB3:**

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
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	0.000	1.00	0.00
SER63	HB2	1.00	0.000	1.00	0.00
SER63	HB3	1.00	0.000	1.00	0.00
SER63	H	1.00	0.000	1.00	0.00
VAL64	H	1.00	0.000	1.00	0.00

**3.63.7 Detailed Probabilities of SER63H:**

Overall probability: 1.000

Overall confidence: 0.917

**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
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**

## 3.63 SER(63)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS62	HA	1.00	0.000	1.00	0.00
LYS62	HB2	1.00	0.000	1.00	0.00
LYS62	HB3	1.00	0.000	1.00	0.00
LYS62	HG2	0.97	0.000	1.00	0.00
LYS62	HG3	0.96	0.000	1.00	0.00
LYS62	H	1.00	0.000	1.00	0.00
LYS62	HD2	0.59	0.000	1.00	0.00
SER63	HA	1.00	0.000	1.00	0.00
SER63	HB2	1.00	0.000	1.00	0.00
SER63	HB3	1.00	0.000	1.00	0.00
SER63	H	1.00	0.000	1.00	0.00
VAL64	H	1.00	0.000	1.00	0.00

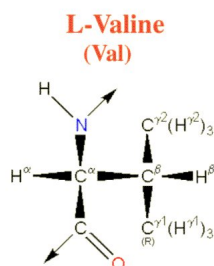
**3.64 VAL(64)**

Figure 54: Image from the BMRB

Residue probability: 0.935

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	0.750	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	1.000	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	0.913	0.917
HA 3.64.6	4.760	4.178	0.599	0.778	1.000
HB 3.64.7	1.675	1.980	0.322	1.000	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	1.000	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: 0.750

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER63	0.00	1.00
VAL64	1.00	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	0.226	0.00	0.00
VAL64	HA	1.00	0.000	1.00	0.00
VAL64	HB	1.00	0.000	1.00	0.00
VAL64	HG11	1.00	0.000	1.00	0.00
VAL64	HG21	1.00	0.000	1.00	0.00
VAL64	H	1.00	0.000	1.00	0.00
PHE65	HA	1.00	0.590	0.00	0.00
PHE65	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
VAL64	HB	1.00	0.000	1.00	0.00
VAL64	HG11	1.00	0.000	1.00	0.00
VAL64	HG21	1.00	0.000	1.00	0.00
VAL64	H	1.00	0.000	1.00	0.00
PHE65	H	1.00	0.000	1.00	0.00

**3.64.3 Detailed Probabilities of VAL64CG1:**

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	0.000	1.00	0.00
VAL64	HB	1.00	0.000	1.00	0.00
VAL64	HG11	1.00	0.000	1.00	0.00
VAL64	HG21	1.00	0.000	1.00	0.00
VAL64	H	1.00	0.000	1.00	0.00
PHE65	H	0.98	0.000	1.00	0.00

**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	0.000	1.00	0.00
VAL64	HB	1.00	0.000	1.00	0.00
VAL64	HG11	1.00	0.000	1.00	0.00
VAL64	HG21	1.00	0.000	1.00	0.00
VAL64	H	1.00	0.000	1.00	0.00

**3.64.5 Detailed Probabilities of VAL64N:**

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	0.000	1.00	0.00
SER63	HB2	1.00	0.000	1.00	0.00
SER63	HB3	1.00	0.000	1.00	0.00
SER63	H	1.00	0.000	1.00	0.00
VAL64	HA	1.00	0.000	1.00	0.00
VAL64	HB	1.00	0.000	1.00	0.00
VAL64	HG11	1.00	0.000	1.00	0.00
VAL64	HG21	1.00	0.000	1.00	0.00
VAL64	H	1.00	0.000	1.00	0.00
PHE65	HA	0.96	0.364	0.04	0.00
PHE65	H	1.00	0.000	1.00	0.00

**3.64.6 Detailed Probabilities of VAL64HA:**

Overall probability: 0.778

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER63	0.00	1.00
VAL64	1.00	1.00
PHE65	0.67	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	0.226	0.00	0.00
VAL64	HA	1.00	0.000	1.00	0.00
VAL64	HB	1.00	0.000	1.00	0.00
VAL64	HG11	1.00	0.000	1.00	0.00
VAL64	HG21	1.00	0.000	1.00	0.00
VAL64	H	1.00	0.000	1.00	0.00
PHE65	HA	1.00	0.261	0.00	0.00
PHE65	H	1.00	0.000	1.00	0.00
PHE65	HB2	0.52	0.025	1.00	0.00

**3.64.7 Detailed Probabilities of VAL64HB:**

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	0.000	1.00	0.00
VAL64	HB	1.00	0.000	1.00	0.00
VAL64	HG11	1.00	0.000	1.00	0.00
VAL64	HG21	1.00	0.000	1.00	0.00
VAL64	H	1.00	0.000	1.00	0.00
PHE65	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
VAL64	HB	1.00	0.000	1.00	0.00
VAL64	HG11	1.00	0.000	1.00	0.00
VAL64	HG21	1.00	0.000	1.00	0.00
VAL64	H	1.00	0.000	1.00	0.00
PHE65	H	0.98	0.000	1.00	0.00

**3.64.9 Detailed Probabilities of VAL64HG21:**

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	0.000	1.00	0.00
VAL64	HB	1.00	0.000	1.00	0.00
VAL64	HG11	1.00	0.000	1.00	0.00
VAL64	HG21	1.00	0.000	1.00	0.00
VAL64	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
SER63	HB2	1.00	0.000	1.00	0.00
SER63	HB3	1.00	0.000	1.00	0.00
SER63	H	1.00	0.000	1.00	0.00
VAL64	HA	1.00	0.000	1.00	0.00
VAL64	HB	1.00	0.000	1.00	0.00
VAL64	HG11	1.00	0.000	1.00	0.00
VAL64	HG21	1.00	0.000	1.00	0.00
VAL64	H	1.00	0.000	1.00	0.00
PHE65	HA	0.96	0.434	0.04	0.00
PHE65	H	1.00	0.000	1.00	0.00

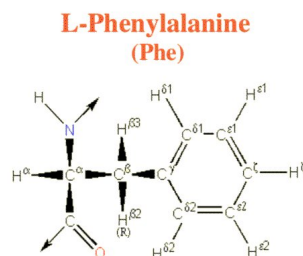


Figure 55: Image from the BMRB

**Residue probability:** 0.928  
**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	0.731	1.000
CB 3.65.2	42.896	40.078	3.616	1.000	1.000
CD1 3.65.3	131.911	131.234	9.579	0.889	1.000
CD2 3.65.4	131.960	131.352	9.581	0.891	1.000
CE1 3.65.5	130.694	130.599	3.219	1.000	1.000
CE2 3.65.6	131.063	130.633	2.839	0.857	1.000
CZ 3.65.7	129.603	129.042	3.448	1.000	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	0.704	1.000
HB2 3.65.10	3.232	2.980	0.399	1.000	1.000
HB3 3.65.11	3.037	2.916	0.434	0.875	1.000
HD1 3.65.12	7.254	7.037	0.347	1.000	1.000
HD2 3.65.13	7.254	7.022	0.417	1.000	1.000
HE1 3.65.14	7.286	7.046	0.417	1.000	1.000
HE2 3.65.15	7.286	7.043	0.400	1.000	1.000
HZ 3.65.16	7.272	6.984	1.598	1.000	1.000
H 3.65.17	9.082	8.375	0.710	0.835	1.000

**3.65.1 Detailed Probabilities of PHE65CA:**

**Overall probability:** 0.731  
**Overall confidence:** 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL64	0.02	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	0.261	0.00	0.00
VAL64	H	0.96	0.434	0.04	0.00
PHE65	HA	1.00	0.000	1.00	0.00
PHE65	HB2	1.00	0.000	1.00	0.00
PHE65	HB3	1.00	0.000	1.00	0.00
PHE65	HD1	1.00	0.003	1.00	0.00
PHE65	HD2	1.00	0.003	1.00	0.00
PHE65	H	1.00	0.000	1.00	0.00
PHE65	HE1	0.74	0.029	1.00	0.00
PHE66	HA	1.00	0.157	0.00	0.00
PHE66	H	1.00	0.000	1.00	0.00

**3.65.2 Detailed Probabilities of PHE65CB:**

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

**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	0.000	1.00	0.00
PHE65	HB2	1.00	0.000	1.00	0.00
PHE65	HB3	1.00	0.000	1.00	0.00
PHE65	HD1	1.00	0.003	1.00	0.00
PHE65	HD2	1.00	0.003	1.00	0.00
PHE65	HE2	1.00	0.029	1.00	0.00
PHE65	H	1.00	0.000	1.00	0.00
PHE65	HE1	0.90	0.029	1.00	0.00
PHE66	H	1.00	0.000	1.00	0.00

## 3.65.3 Detailed Probabilities of PHE65CD1:

Overall probability: 0.889

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
PHE65	0.89	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	0.000	1.00	0.00
PHE65	HB2	1.00	0.000	1.00	0.00
PHE65	HB3	1.00	0.000	1.00	0.00
PHE65	HD1	1.00	0.003	1.00	0.00
PHE65	HD2	1.00	0.003	1.00	0.00
PHE65	HE1	1.00	0.003	1.00	0.00
PHE65	HE2	1.00	0.003	1.00	0.00
PHE65	HZ	1.00	0.001	1.00	0.00
PHE65	H	1.00	1.180	0.00	0.00

## 3.65.4 Detailed Probabilities of PHE65CD2:

Overall probability: 0.891

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE65	0.89	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	0.000	1.00	0.00
PHE65	HB2	1.00	0.000	1.00	0.00
PHE65	HB3	1.00	0.000	1.00	0.00
PHE65	HD1	1.00	0.003	1.00	0.00
PHE65	HD2	1.00	0.003	1.00	0.00
PHE65	HE1	1.00	0.003	1.00	0.00
PHE65	HE2	1.00	0.003	1.00	0.00
PHE65	HZ	1.00	0.001	1.00	0.00
PHE65	H	0.99	1.180	0.01	0.00

**3.65.5 Detailed Probabilities of PHE65CE1:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE65	1.00	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	0.003	1.00	0.00
PHE65	HD2	1.00	0.003	1.00	0.00
PHE65	HE1	1.00	0.003	1.00	0.00
PHE65	HE2	1.00	0.003	1.00	0.00
PHE65	HZ	1.00	0.001	1.00	0.00
PHE65	HB2	0.90	0.014	1.00	0.00

**3.65.6 Detailed Probabilities of PHE65CE2:**

Overall probability: 0.857

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE65	0.86	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	0.014	1.00	0.00
PHE65	HB3	1.00	0.181	0.00	0.00
PHE65	HD1	1.00	0.003	1.00	0.00
PHE65	HD2	1.00	0.003	1.00	0.00
PHE65	HE1	1.00	0.003	1.00	0.00
PHE65	HE2	1.00	0.003	1.00	0.00
PHE65	HZ	1.00	0.001	1.00	0.00

**3.65.7 Detailed Probabilities of PHE65CZ:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE65	1.00	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	0.003	1.00	0.00
PHE65	HD2	1.00	0.003	1.00	0.00
PHE65	HE1	1.00	0.003	1.00	0.00
PHE65	HE2	1.00	0.003	1.00	0.00
PHE65	HZ	1.00	0.001	1.00	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	0.000	1.00	0.00
VAL64	HB	1.00	0.000	1.00	0.00
VAL64	HG11	0.98	0.000	1.00	0.00
VAL64	H	1.00	0.000	1.00	0.00
VAL64	HG21	0.95	0.000	1.00	0.00
PHE65	HA	1.00	0.000	1.00	0.00
PHE65	HB2	1.00	0.000	1.00	0.00
PHE65	HB3	1.00	0.000	1.00	0.00
PHE65	HD1	1.00	0.003	1.00	0.00
PHE65	HD2	0.99	0.003	1.00	0.00
PHE65	H	1.00	0.000	1.00	0.00
PHE66	H	1.00	0.000	1.00	0.00
PHE66	HB2	0.56	0.027	1.00	0.00

**3.65.9 Detailed Probabilities of PHE65HA:**

Overall probability: 0.704

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL64	0.02	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	0.590	0.00	0.00
VAL64	H	0.96	0.364	0.04	0.00
PHE65	HA	1.00	0.000	1.00	0.00
PHE65	HB2	1.00	0.000	1.00	0.00
PHE65	HB3	1.00	0.000	1.00	0.00
PHE65	HD1	1.00	0.000	1.00	0.00
PHE65	HD2	1.00	0.000	1.00	0.00
PHE65	H	1.00	0.000	1.00	0.00
PHE66	HA	1.00	0.157	0.00	0.00
PHE66	H	1.00	0.000	1.00	0.00

**3.65.10 Detailed Probabilities of PHE65HB2:**

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

**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	0.000	1.00	0.00
PHE65	HB2	1.00	0.000	1.00	0.00
PHE65	HB3	1.00	0.000	1.00	0.00
PHE65	HD1	1.00	0.000	1.00	0.00
PHE65	HD2	1.00	0.000	1.00	0.00
PHE65	HE2	1.00	0.014	1.00	0.00
PHE65	H	1.00	0.000	1.00	0.00
PHE65	HE1	0.90	0.014	1.00	0.00
PHE66	H	1.00	0.000	1.00	0.00
PHE66	HA	0.59	0.027	1.00	0.00

## 3.65.11 Detailed Probabilities of PHE65HB3:

Overall probability: 0.875

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
PHE65	0.86	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	0.000	1.00	0.00
PHE65	HB2	1.00	0.000	1.00	0.00
PHE65	HB3	1.00	0.000	1.00	0.00
PHE65	HD1	1.00	0.000	1.00	0.00
PHE65	HD2	1.00	0.000	1.00	0.00
PHE65	HE2	1.00	0.181	0.00	0.00
PHE65	H	1.00	0.000	1.00	0.00
PHE66	H	1.00	0.000	1.00	0.00

## 3.65.12 Detailed Probabilities of PHE65HD1:

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE65	1.00	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	0.003	1.00	0.00
PHE65	HB2	1.00	0.003	1.00	0.00
PHE65	HB3	1.00	0.003	1.00	0.00
PHE65	HD1	1.00	0.003	1.00	0.00
PHE65	HD2	1.00	0.003	1.00	0.00
PHE65	HE1	1.00	0.003	1.00	0.00
PHE65	HE2	1.00	0.003	1.00	0.00
PHE65	HZ	1.00	0.003	1.00	0.00
PHE65	H	1.00	0.003	1.00	0.00

**3.65.13 Detailed Probabilities of PHE65HD2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE65	1.00	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	0.003	1.00	0.00
PHE65	HB2	1.00	0.003	1.00	0.00
PHE65	HB3	1.00	0.003	1.00	0.00
PHE65	HD1	1.00	0.003	1.00	0.00
PHE65	HD2	1.00	0.003	1.00	0.00
PHE65	HE1	1.00	0.003	1.00	0.00
PHE65	HE2	1.00	0.003	1.00	0.00
PHE65	HZ	1.00	0.003	1.00	0.00
PHE65	H	0.99	0.003	1.00	0.00

**3.65.14 Detailed Probabilities of PHE65HE1:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE65	1.00	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	0.003	1.00	0.00
PHE65	HD2	1.00	0.003	1.00	0.00
PHE65	HE1	1.00	0.003	1.00	0.00
PHE65	HE2	1.00	0.003	1.00	0.00
PHE65	HZ	1.00	0.003	1.00	0.00
PHE65	HA	0.74	0.029	1.00	0.00
PHE65	HB2	0.90	0.029	1.00	0.00
PHE65	HB3	0.89	0.029	1.00	0.00

**3.65.15 Detailed Probabilities of PHE65HE2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE65	1.00	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	0.029	1.00	0.00
PHE65	HB3	1.00	0.029	1.00	0.00
PHE65	HD1	1.00	0.003	1.00	0.00
PHE65	HD2	1.00	0.003	1.00	0.00
PHE65	HE1	1.00	0.003	1.00	0.00
PHE65	HE2	1.00	0.003	1.00	0.00
PHE65	HZ	1.00	0.003	1.00	0.00

**3.65.16 Detailed Probabilities of PHE65HZ:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE65	1.00	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	0.001	1.00	0.00
PHE65	HD2	1.00	0.001	1.00	0.00
PHE65	HE1	1.00	0.001	1.00	0.00
PHE65	HE2	1.00	0.001	1.00	0.00
PHE65	HZ	1.00	0.001	1.00	0.00

**3.65.17 Detailed Probabilities of PHE65H:**

Overall probability: 0.835

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL64	1.00	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	0.000	1.00	0.00
VAL64	HB	1.00	0.000	1.00	0.00
VAL64	HG11	0.98	0.000	1.00	0.00
VAL64	H	1.00	0.000	1.00	0.00
VAL64	HG21	0.95	0.000	1.00	0.00
PHE65	HA	1.00	0.000	1.00	0.00
PHE65	HB2	1.00	0.000	1.00	0.00
PHE65	HB3	1.00	0.000	1.00	0.00
PHE65	HD1	1.00	1.180	0.00	0.00
PHE65	HD2	0.99	1.180	0.01	0.00
PHE65	H	1.00	0.000	1.00	0.00
PHE66	H	1.00	0.000	1.00	0.00

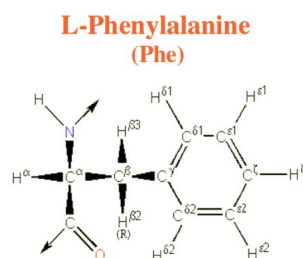


Figure 56: Image from the BMRB

**Residue probability:** 0.930  
**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	0.923	1.000
HA 3.66.9	5.507	4.625	1.237	0.818	1.000
HB2 3.66.10	3.205	2.980	0.399	1.000	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	1.000	1.000
HD2 3.66.13	7.148	7.022	0.417	1.000	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	0.909	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	0.157	0.00	0.00
PHE65	HB2	0.59	0.027	1.00	0.00
PHE66	HA	1.00	0.000	1.00	0.00
PHE66	HB2	1.00	0.000	1.00	0.00
PHE66	HB3	1.00	0.000	1.00	0.00
PHE66	HD1	1.00	0.000	1.00	0.00
PHE66	HD2	1.00	0.000	1.00	0.00
PHE66	H	1.00	0.000	1.00	0.00
PHE66	HE1	0.74	0.000	1.00	0.00
GLY67	HA2	1.00	0.550	0.00	0.00
GLY67	HA3	1.00	0.024	1.00	0.00
GLY67	H	1.00	0.000	1.00	0.00

**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
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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE66	HA	1.00	0.000	1.00	0.00
PHE66	HB2	1.00	0.000	1.00	0.00
PHE66	HB3	1.00	0.000	1.00	0.00
PHE66	HD1	1.00	0.000	1.00	0.00
PHE66	HD2	1.00	0.000	1.00	0.00
PHE66	HE2	1.00	0.195	0.00	0.00
PHE66	H	1.00	0.000	1.00	0.00
GLY67	H	1.00	0.000	1.00	0.00

## 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	0.000	1.00	0.00
PHE66	HB2	1.00	0.000	1.00	0.00
PHE66	HB3	1.00	0.000	1.00	0.00
PHE66	HD1	1.00	0.000	1.00	0.00
PHE66	HD2	1.00	0.000	1.00	0.00
PHE66	HE1	1.00	0.000	1.00	0.00
PHE66	HE2	1.00	0.000	1.00	0.00
PHE66	HZ	1.00	0.000	1.00	0.00
PHE66	H	1.00	0.000	1.00	0.00

## 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	0.000	1.00	0.00
PHE66	HB2	1.00	0.000	1.00	0.00
PHE66	HB3	1.00	0.000	1.00	0.00
PHE66	HD1	1.00	0.000	1.00	0.00
PHE66	HD2	1.00	0.000	1.00	0.00
PHE66	HE1	1.00	0.000	1.00	0.00
PHE66	HE2	1.00	0.000	1.00	0.00
PHE66	HZ	1.00	0.000	1.00	0.00
PHE66	H	0.99	0.000	1.00	0.00

**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	0.000	1.00	0.00
PHE66	HD2	1.00	0.000	1.00	0.00
PHE66	HE1	1.00	0.000	1.00	0.00
PHE66	HE2	1.00	0.000	1.00	0.00
PHE66	HZ	1.00	0.000	1.00	0.00
PHE66	HA	0.74	0.000	1.00	0.00
PHE66	HB2	0.90	0.000	1.00	0.00

**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	0.000	1.00	0.00
PHE66	HB3	1.00	0.126	0.00	0.00
PHE66	HD1	1.00	0.000	1.00	0.00
PHE66	HD2	1.00	0.000	1.00	0.00
PHE66	HE1	1.00	0.000	1.00	0.00
PHE66	HE2	1.00	0.000	1.00	0.00
PHE66	HZ	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
PHE66	HD2	1.00	0.000	1.00	0.00
PHE66	HE1	1.00	0.000	1.00	0.00
PHE66	HE2	1.00	0.000	1.00	0.00
PHE66	HZ	1.00	0.000	1.00	0.00

**3.66.8 Detailed Probabilities of PHE66N:**

Overall probability: 0.923

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE65	1.00	1.00
PHE66	1.00	1.00
GLY67	0.00	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	0.000	1.00	0.00
PHE65	HB2	1.00	0.000	1.00	0.00
PHE65	HB3	1.00	0.000	1.00	0.00
PHE65	H	1.00	0.000	1.00	0.00
PHE65	HD1	0.79	0.003	1.00	0.00
PHE65	HD2	0.70	0.003	1.00	0.00
PHE66	HA	1.00	0.000	1.00	0.00
PHE66	HB2	1.00	0.000	1.00	0.00
PHE66	HB3	1.00	0.000	1.00	0.00
PHE66	HD1	1.00	0.000	1.00	0.00
PHE66	HD2	0.99	0.000	1.00	0.00
PHE66	H	1.00	0.000	1.00	0.00
GLY67	H	1.00	0.176	0.00	0.00

**3.66.9 Detailed Probabilities of PHE66HA:**

Overall probability: 0.818

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE65	0.00	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	0.157	0.00	0.00
PHE66	HA	1.00	0.000	1.00	0.00
PHE66	HB2	1.00	0.000	1.00	0.00
PHE66	HB3	1.00	0.000	1.00	0.00
PHE66	HD1	1.00	0.000	1.00	0.00
PHE66	HD2	1.00	0.000	1.00	0.00
PHE66	H	1.00	0.000	1.00	0.00
PHE66	HE1	0.74	0.000	1.00	0.00
GLY67	HA2	1.00	0.012	1.00	0.00
GLY67	HA3	1.00	0.765	0.00	0.00
GLY67	H	1.00	0.000	1.00	0.00

**3.66.10 Detailed Probabilities of PHE66HB2:**

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

**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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE66	HA	1.00	0.000	1.00	0.00
PHE66	HB2	1.00	0.000	1.00	0.00
PHE66	HB3	1.00	0.000	1.00	0.00
PHE66	HD1	1.00	0.000	1.00	0.00
PHE66	HD2	1.00	0.000	1.00	0.00
PHE66	HE2	1.00	0.000	1.00	0.00
PHE66	H	1.00	0.000	1.00	0.00
PHE66	HE1	0.90	0.000	1.00	0.00
GLY67	H	1.00	0.000	1.00	0.00

## 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	0.000	1.00	0.00
PHE66	HB2	1.00	0.000	1.00	0.00
PHE66	HB3	1.00	0.000	1.00	0.00
PHE66	HD1	1.00	0.000	1.00	0.00
PHE66	HD2	1.00	0.000	1.00	0.00
PHE66	HE2	1.00	0.126	0.00	0.00
PHE66	H	1.00	0.000	1.00	0.00
GLY67	H	1.00	0.000	1.00	0.00

## 3.66.12 Detailed Probabilities of PHE66HD1:

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	0.000	1.00	0.00
PHE66	HB2	1.00	0.000	1.00	0.00
PHE66	HB3	1.00	0.000	1.00	0.00
PHE66	HD1	1.00	0.000	1.00	0.00
PHE66	HD2	1.00	0.000	1.00	0.00
PHE66	HE1	1.00	0.000	1.00	0.00
PHE66	HE2	1.00	0.000	1.00	0.00
PHE66	HZ	1.00	0.000	1.00	0.00
PHE66	H	1.00	0.000	1.00	0.00

**3.66.13 Detailed Probabilities of PHE66HD2:**

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**

## 3.66 PHE(66)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE66	HA	1.00	0.000	1.00	0.00
PHE66	HB2	1.00	0.000	1.00	0.00
PHE66	HB3	1.00	0.000	1.00	0.00
PHE66	HD1	1.00	0.000	1.00	0.00
PHE66	HD2	1.00	0.000	1.00	0.00
PHE66	HE1	1.00	0.000	1.00	0.00
PHE66	HE2	1.00	0.000	1.00	0.00
PHE66	HZ	1.00	0.000	1.00	0.00
PHE66	H	0.99	0.000	1.00	0.00

## 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	0.000	1.00	0.00
PHE66	HD2	1.00	0.000	1.00	0.00
PHE66	HE1	1.00	0.000	1.00	0.00
PHE66	HE2	1.00	0.000	1.00	0.00
PHE66	HZ	1.00	0.000	1.00	0.00
PHE66	HA	0.74	0.000	1.00	0.00

## 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	0.195	0.00	0.00
PHE66	HB3	1.00	0.195	0.00	0.00
PHE66	HD1	1.00	0.000	1.00	0.00
PHE66	HD2	1.00	0.000	1.00	0.00
PHE66	HE1	1.00	0.000	1.00	0.00
PHE66	HE2	1.00	0.000	1.00	0.00
PHE66	HZ	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
PHE66	HD2	1.00	0.000	1.00	0.00
PHE66	HE1	1.00	0.000	1.00	0.00
PHE66	HE2	1.00	0.000	1.00	0.00
PHE66	HZ	1.00	0.000	1.00	0.00

**3.66.17 Detailed Probabilities of PHE66H:**

Overall probability: 0.909

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE65	0.75	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	0.000	1.00	0.00
PHE65	HB2	1.00	0.000	1.00	0.00
PHE65	HB3	1.00	0.231	0.00	0.00
PHE65	H	1.00	0.000	1.00	0.00
PHE66	HA	1.00	0.000	1.00	0.00
PHE66	HB2	1.00	0.000	1.00	0.00
PHE66	HB3	1.00	0.000	1.00	0.00
PHE66	HD1	1.00	0.000	1.00	0.00
PHE66	HD2	0.99	0.000	1.00	0.00
PHE66	H	1.00	0.000	1.00	0.00
GLY67	H	1.00	0.000	1.00	0.00

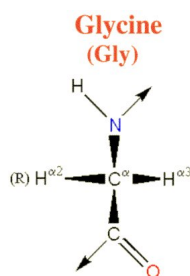
**3.67 GLY(67)**

Figure 57: Image from the BMRB

Residue probability: 0.762

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	0.875	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	0.500	1.000
HA3 3.67.4	4.742	3.897	0.390	0.857	1.000
H 3.67.5	8.558	8.343	0.939	0.668	1.000

**3.67.1 Detailed Probabilities of GLY67CA:**

Overall probability: 0.875

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE66	1.00	1.00
GLY67	1.00	1.00
PRO68	0.75	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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE66	HA	1.00	0.012	1.00	0.00
GLY67	HA2	1.00	0.000	1.00	0.00
GLY67	HA3	1.00	0.000	1.00	0.00
GLY67	H	1.00	0.000	1.00	0.00
PRO68	HA	1.00	0.279	0.00	0.00
PRO68	HD2	1.00	0.001	1.00	0.00
PRO68	HD3	1.00	0.000	1.00	0.00
PRO68	HG3	0.85	0.003	1.00	0.00

## 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	0.000	1.00	0.00
PHE66	HB2	1.00	0.000	1.00	0.00
PHE66	HB3	1.00	0.000	1.00	0.00
PHE66	H	1.00	0.000	1.00	0.00
PHE66	HD1	0.77	0.000	1.00	0.00
PHE66	HD2	0.63	0.000	1.00	0.00
GLY67	HA2	1.00	0.000	1.00	0.00
GLY67	HA3	1.00	0.000	1.00	0.00
GLY67	H	1.00	0.000	1.00	0.00
PRO68	HD2	0.99	0.003	1.00	0.00
PRO68	HD3	0.99	0.059	0.01	0.00

**3.67.3 Detailed Probabilities of GLY67HA2:**

Overall probability: 0.500

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE66	0.00	1.00
GLY67	1.00	1.00
PRO68	0.25	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	0.550	0.00	0.00
GLY67	HA2	1.00	0.000	1.00	0.00
GLY67	HA3	1.00	0.000	1.00	0.00
GLY67	H	1.00	0.000	1.00	0.00
PRO68	HA	1.00	0.058	0.00	0.00
PRO68	HD2	1.00	0.059	0.00	0.00
PRO68	HD3	1.00	0.059	0.00	0.00
PRO68	HG2	0.84	0.023	1.00	0.00

**3.67.4 Detailed Probabilities of GLY67HA3:**

Overall probability: 0.857

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE66	1.00	1.00
GLY67	1.00	1.00
PRO68	0.67	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	0.024	1.00	0.00
GLY67	HA2	1.00	0.000	1.00	0.00
GLY67	HA3	1.00	0.000	1.00	0.00
GLY67	H	1.00	0.000	1.00	0.00
PRO68	HA	1.00	0.279	0.00	0.00
PRO68	HD2	1.00	0.011	1.00	0.00
PRO68	HD3	1.00	0.008	1.00	0.00

**3.67.5 Detailed Probabilities of GLY67H:**

Overall probability: 0.668

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE66	0.75	1.00
GLY67	1.00	1.00
PRO68	0.01	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	0.000	1.00	0.00
PHE66	HB2	1.00	0.000	1.00	0.00
PHE66	HB3	1.00	0.000	1.00	0.00
PHE66	H	1.00	0.176	0.00	0.00
GLY67	HA2	1.00	0.000	1.00	0.00
GLY67	HA3	1.00	0.000	1.00	0.00
GLY67	H	1.00	0.000	1.00	0.00
PRO68	HD2	0.99	3.670	0.01	0.00
PRO68	HD3	0.99	3.682	0.01	0.00

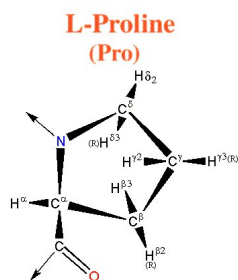


Figure 58: Image from the BMRB

**Residue probability:** 0.898  
**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	0.700	0.909
CB 3.68.2	31.942	33.632	13.629	1.000	0.875
CG 3.68.3	27.601	28.412	13.801	1.000	1.000
CD 3.68.4	49.045	49.797	3.175	0.801	1.000
N	NA	—	—	0.000	0.000
HA 3.68.5	4.463	4.332	0.427	0.700	0.909
HB2 3.68.6	1.875	2.099	0.501	0.877	0.889
HB3 3.68.7	2.314	2.052	0.596	1.000	0.875
HG2 3.68.8	2.084	1.927	0.364	1.000	1.000
HG3 3.68.9	1.888	1.907	0.417	1.000	1.000
HD2 3.68.10	3.500	3.640	0.682	1.000	1.000
HD3 3.68.11	3.827	3.558	0.522	0.801	1.000

**3.68.1 Detailed Probabilities of PRO68CA:**

**Overall probability:** 0.700  
**Overall confidence:** 0.909

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLY67	0.00	1.00
PRO68	1.00	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	0.058	0.00	0.00
GLY67	HA3	1.00	0.279	0.00	0.00
PRO68	HA	1.00	0.000	1.00	0.00
PRO68	HB2	1.00	0.000	1.00	0.00
PRO68	HB3	1.00	0.000	1.00	0.00
PRO68	HG2	1.00	0.000	1.00	0.00
PRO68	HG3	1.00	0.000	1.00	0.00
PRO68	HD2	1.00	0.006	1.00	0.00
PRO68	HD3	1.00	0.001	1.00	0.00
ASP69	HA	1.00	0.241	0.00	0.00

**3.68.2 Detailed Probabilities of PRO68CB:**

Overall probability: 1.000

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO68	1.00	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	0.000	1.00	0.00
PRO68	HB2	1.00	0.000	1.00	0.00
PRO68	HB3	1.00	0.000	1.00	0.00
PRO68	HG2	1.00	0.000	1.00	0.00
PRO68	HG3	1.00	0.000	1.00	0.00
PRO68	HD2	1.00	0.000	1.00	0.00
PRO68	HD3	1.00	0.000	1.00	0.00

**3.68.3 Detailed Probabilities of PRO68CG:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO68	1.00	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	0.000	1.00	0.00
PRO68	HB2	1.00	0.000	1.00	0.00
PRO68	HB3	1.00	0.000	1.00	0.00
PRO68	HG2	1.00	0.000	1.00	0.00
PRO68	HG3	1.00	0.000	1.00	0.00
PRO68	HD2	1.00	0.000	1.00	0.00
PRO68	HD3	1.00	0.000	1.00	0.00

**3.68.4 Detailed Probabilities of PRO68CD:**

Overall probability: 0.801

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLY67	0.34	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	0.059	0.00	0.00
GLY67	HA3	1.00	0.011	1.00	0.00
GLY67	H	0.99	3.670	0.01	0.00
PRO68	HA	1.00	0.000	1.00	0.00
PRO68	HB2	1.00	0.000	1.00	0.00
PRO68	HB3	1.00	0.000	1.00	0.00
PRO68	HG2	1.00	0.000	1.00	0.00
PRO68	HG3	1.00	0.000	1.00	0.00
PRO68	HD2	1.00	0.000	1.00	0.00
PRO68	HD3	1.00	0.000	1.00	0.00

**3.68.5 Detailed Probabilities of PRO68HA:**

Overall probability: 0.700

Overall confidence: 0.909

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLY67	0.00	1.00
PRO68	1.00	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	0.279	0.00	0.00
GLY67	HA3	1.00	0.279	0.00	0.00
PRO68	HA	1.00	0.000	1.00	0.00
PRO68	HB2	1.00	0.000	1.00	0.00
PRO68	HB3	1.00	0.000	1.00	0.00
PRO68	HG2	1.00	0.000	1.00	0.00
PRO68	HG3	1.00	0.000	1.00	0.00
PRO68	HD2	1.00	0.000	1.00	0.00
PRO68	HD3	1.00	0.000	1.00	0.00
ASP69	HA	1.00	0.219	0.00	0.00

**3.68.6 Detailed Probabilities of PRO68HB2:**

Overall probability: 0.877

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO68	1.00	1.00
ASP69	0.01	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	0.000	1.00	0.00
PRO68	HB2	1.00	0.000	1.00	0.00
PRO68	HB3	1.00	0.000	1.00	0.00
PRO68	HG2	1.00	0.000	1.00	0.00
PRO68	HG3	1.00	0.000	1.00	0.00
PRO68	HD2	1.00	0.000	1.00	0.00
PRO68	HD3	1.00	0.000	1.00	0.00
ASP69	HA	0.99	0.731	0.01	0.00

**3.68.7 Detailed Probabilities of PRO68HB3:**

Overall probability: 1.000

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO68	1.00	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	0.00
PRO68	HB2	1.00	0.000	1.00	0.00
PRO68	HB3	1.00	0.000	1.00	0.00
PRO68	HG2	1.00	0.000	1.00	0.00
PRO68	HG3	1.00	0.000	1.00	0.00
PRO68	HD2	1.00	0.000	1.00	0.00
PRO68	HD3	1.00	0.000	1.00	0.00

**3.68.8 Detailed Probabilities of PRO68HG2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO68	1.00	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	0.000	1.00	0.00
PRO68	HB2	1.00	0.000	1.00	0.00
PRO68	HB3	1.00	0.000	1.00	0.00
PRO68	HG2	1.00	0.000	1.00	0.00
PRO68	HG3	1.00	0.000	1.00	0.00
PRO68	HD2	1.00	0.000	1.00	0.00
PRO68	HD3	1.00	0.000	1.00	0.00

**3.68.9 Detailed Probabilities of PRO68HG3:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO68	1.00	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	0.000	1.00	0.00
PRO68	HB2	1.00	0.000	1.00	0.00
PRO68	HB3	1.00	0.000	1.00	0.00
PRO68	HG2	1.00	0.000	1.00	0.00
PRO68	HG3	1.00	0.000	1.00	0.00
PRO68	HD2	1.00	0.000	1.00	0.00
PRO68	HD3	1.00	0.000	1.00	0.00

**3.68.10 Detailed Probabilities of PRO68HD2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLY67	1.00	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	0.001	1.00	0.00
GLY67	HA3	1.00	0.030	1.00	0.00
GLY67	H	0.99	0.003	1.00	0.00
PRO68	HA	1.00	0.006	1.00	0.00
PRO68	HB2	1.00	0.000	1.00	0.00
PRO68	HB3	1.00	0.000	1.00	0.00
PRO68	HG2	1.00	0.000	1.00	0.00
PRO68	HG3	1.00	0.000	1.00	0.00
PRO68	HD2	1.00	0.000	1.00	0.00
PRO68	HD3	1.00	0.000	1.00	0.00

**3.68.11 Detailed Probabilities of PRO68HD3:**

Overall probability: 0.801

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLY67	0.34	1.00
PRO68	1.00	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	0.000	1.00	0.00
GLY67	HA3	1.00	0.059	0.00	0.00
GLY67	H	0.99	0.059	0.01	0.00
PRO68	HA	1.00	0.001	1.00	0.00
PRO68	HB2	1.00	0.000	1.00	0.00
PRO68	HB3	1.00	0.000	1.00	0.00
PRO68	HG2	1.00	0.000	1.00	0.00
PRO68	HG3	1.00	0.000	1.00	0.00
PRO68	HD2	1.00	0.000	1.00	0.00
PRO68	HD3	1.00	0.000	1.00	0.00

**3.69 ASP(69)**

Figure 59: Image from the BMRB

Residue probability: 0.805

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	0.573	0.778
CB 3.69.2	41.452	40.949	3.070	0.750	0.667
N	NA	—	—	0.000	0.000
HD2	NA	—	—	0.000	0.000
HA 3.69.3	4.704	4.587	0.329	0.700	0.778
HB2 3.69.4	2.924	2.708	0.282	1.000	0.667
HB3 3.69.5	2.606	2.654	0.285	1.000	0.667
H	NA	—	—	0.000	0.000

**3.69.1 Detailed Probabilities of ASP69CA:**

Overall probability: 0.573

Overall confidence: 0.778

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO68	0.01	1.00
ASP69	1.00	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	0.219	0.00	0.00
PRO68	HB2	0.99	0.731	0.01	0.00
ASP69	HA	1.00	0.000	1.00	0.00
ASP69	HB2	1.00	0.000	1.00	0.00
ASP69	HB3	1.00	0.000	1.00	0.00
SER70	HA	1.00	0.394	0.00	0.00
SER70	H	1.00	0.000	1.00	0.00

**3.69.2 Detailed Probabilities of ASP69CB:**

Overall probability: 0.750

Overall confidence: 0.667

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASP69	1.00	0.60
SER70	0.00	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	0.000	1.00	0.00
ASP69	HB2	1.00	0.000	1.00	0.00
ASP69	HB3	1.00	0.000	1.00	0.00
SER70	H	1.00	0.650	0.00	0.00

**3.69.3 Detailed Probabilities of ASP69HA:**

Overall probability: 0.700

Overall confidence: 0.778

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO68	0.45	1.00
ASP69	1.00	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	0.241	0.00	0.00
PRO68	HB2	0.99	0.031	0.90	0.00
ASP69	HA	1.00	0.000	1.00	0.00
ASP69	HB2	1.00	0.000	1.00	0.00
ASP69	HB3	1.00	0.000	1.00	0.00
SER70	HA	1.00	0.394	0.00	0.00
SER70	H	1.00	0.000	1.00	0.00

**3.69.4 Detailed Probabilities of ASP69HB2:**

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
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	0.000	1.00	0.00
ASP69	HB2	1.00	0.000	1.00	0.00
ASP69	HB3	1.00	0.000	1.00	0.00
SER70	H	1.00	0.000	1.00	0.00

**3.69.5 Detailed Probabilities of ASP69HB3:**

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	0.000	1.00	0.00
ASP69	HB2	1.00	0.000	1.00	0.00
ASP69	HB3	1.00	0.000	1.00	0.00
SER70	H	1.00	0.000	1.00	0.00

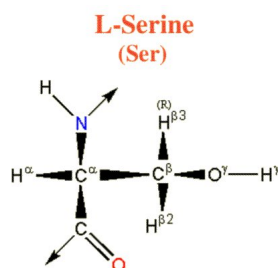


Figure 60: Image from the BMRB

**Residue probability:** 0.883  
**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	0.714	0.875
CB 3.70.2	66.693	63.523	4.288	1.000	0.833
N 3.70.3	109.416	116.135	5.326	1.000	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	1.000	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	0.750	0.800
HG	NA	—	—	0.000	0.000

**3.70.1 Detailed Probabilities of SER70CA:**

**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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP69	HA	1.00	0.394	0.00	0.00
SER70	HA	1.00	0.000	1.00	0.00
SER70	HB2	1.00	0.000	1.00	0.00
SER70	HB3	1.00	0.000	1.00	0.00
SER70	H	1.00	0.000	1.00	0.00
ILE71	HA	1.00	0.070	0.00	0.00
ILE71	H	1.00	0.000	1.00	0.00

**3.70.2 Detailed Probabilities of SER70CB:**

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
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	0.000	1.00	0.00
SER70	HB2	1.00	0.000	1.00	0.00
SER70	HB3	1.00	0.000	1.00	0.00
SER70	H	1.00	0.000	1.00	0.00
ILE71	H	1.00	0.000	1.00	0.00

**3.70.3 Detailed Probabilities of SER70N:**

Overall probability: 1.000

Overall confidence: 0.800

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASP69	1.00	0.75
SER70	1.00	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	0.000	1.00	0.00
ASP69	HB2	1.00	0.000	1.00	0.00
ASP69	HB3	1.00	0.000	1.00	0.00
SER70	HA	1.00	0.000	1.00	0.00
SER70	HB2	1.00	0.000	1.00	0.00
SER70	HB3	1.00	0.000	1.00	0.00
SER70	H	1.00	0.000	1.00	0.00
ILE71	H	1.00	0.000	1.00	0.00

**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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP69	HA	1.00	0.394	0.00	0.00
SER70	HA	1.00	0.000	1.00	0.00
SER70	HB2	1.00	0.000	1.00	0.00
SER70	HB3	1.00	0.000	1.00	0.00
SER70	H	1.00	0.000	1.00	0.00
ILE71	HA	1.00	0.070	0.00	0.00
ILE71	H	1.00	0.000	1.00	0.00

## 3.70.5 Detailed Probabilities of SER70HB2:

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
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	0.000	1.00	0.00
SER70	HB2	1.00	0.000	1.00	0.00
SER70	HB3	1.00	0.000	1.00	0.00
SER70	H	1.00	0.000	1.00	0.00
ILE71	H	1.00	0.000	1.00	0.00

## 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	0.000	1.00	0.00
SER70	HB2	1.00	0.000	1.00	0.00
SER70	HB3	1.00	0.000	1.00	0.00
SER70	H	1.00	0.000	1.00	0.00
ILE71	H	1.00	0.000	1.00	0.00

**3.70.7 Detailed Probabilities of SER70H:**

Overall probability: 0.750

Overall confidence: 0.800

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASP69	0.33	0.75
SER70	1.00	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	0.000	1.00	0.00
ASP69	HB2	1.00	0.650	0.00	0.00
ASP69	HB3	1.00	0.646	0.00	0.00
SER70	HA	1.00	0.000	1.00	0.00
SER70	HB2	1.00	0.000	1.00	0.00
SER70	HB3	1.00	0.000	1.00	0.00
SER70	H	1.00	0.000	1.00	0.00
ILE71	H	1.00	0.000	1.00	0.00

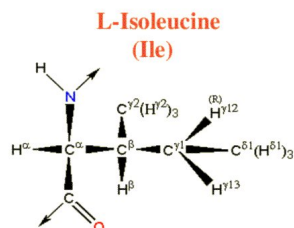


Figure 61: Image from the BMRB

Residue probability: 0.969  
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	0.800	1.000
CB 3.71.2	42.854	38.702	3.945	1.000	1.000
CG1 3.71.3	28.132	27.785	2.037	1.000	1.000
CG2 3.71.4	17.663	17.574	1.928	1.000	1.000
CD1 3.71.5	15.672	13.545	3.646	1.000	1.000
N 3.71.6	120.092	121.467	6.098	1.000	0.917
HA 3.71.7	5.168	4.185	1.403	0.800	1.000
HB 3.71.8	1.761	1.776	0.310	1.000	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	1.000	1.000
HG2 3.71.11	0.942	0.762	0.283	1.000	1.000
HD1 3.71.12	0.703	0.668	0.293	1.000	1.000
H 3.71.13	9.191	8.301	0.685	1.000	0.917

**3.71.1 Detailed Probabilities of ILE71CA:**

Overall probability: 0.800  
Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER70	0.00	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	0.070	0.00	0.00
ILE71	HA	1.00	0.000	1.00	0.00
ILE71	HB	1.00	0.000	1.00	0.00
ILE71	HG12	1.00	0.000	1.00	0.00
ILE71	HG13	1.00	0.000	1.00	0.00
ILE71	HG21	1.00	0.000	1.00	0.00
ILE71	HD11	0.97	0.000	1.00	0.00
ILE71	H	1.00	0.000	1.00	0.00
THR72	HA	1.00	0.048	0.00	0.00
THR72	H	1.00	0.000	1.00	0.00

**3.71.2 Detailed Probabilities of ILE71CB:**

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
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	0.000	1.00	0.00
ILE71	HB	1.00	0.000	1.00	0.00
ILE71	HG12	1.00	0.000	1.00	0.00
ILE71	HG13	1.00	0.000	1.00	0.00
ILE71	HG21	1.00	0.000	1.00	0.00
ILE71	HD11	1.00	0.000	1.00	0.00
ILE71	H	1.00	0.000	1.00	0.00
THR72	H	1.00	0.000	1.00	0.00

## 3.71.3 Detailed Probabilities of ILE71CG1:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
ILE71	1.00	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	0.000	1.00	0.00
ILE71	HB	1.00	0.000	1.00	0.00
ILE71	HG12	1.00	0.000	1.00	0.00
ILE71	HG13	1.00	0.000	1.00	0.00
ILE71	HG21	1.00	0.000	1.00	0.00
ILE71	HD11	1.00	0.000	1.00	0.00
ILE71	H	1.00	0.000	1.00	0.00

## 3.71.4 Detailed Probabilities of ILE71CG2:

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
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	0.000	1.00	0.00
ILE71	HB	1.00	0.000	1.00	0.00
ILE71	HG12	1.00	0.000	1.00	0.00
ILE71	HG13	1.00	0.000	1.00	0.00
ILE71	HG21	1.00	0.000	1.00	0.00
ILE71	HD11	0.99	0.000	1.00	0.00
ILE71	H	1.00	0.000	1.00	0.00
THR72	H	0.99	0.000	1.00	0.00

**3.71.5 Detailed Probabilities of ILE71CD1:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE71	1.00	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	0.000	1.00	0.00
ILE71	HB	1.00	0.000	1.00	0.00
ILE71	HG12	1.00	0.000	1.00	0.00
ILE71	HG13	1.00	0.000	1.00	0.00
ILE71	HG21	0.99	0.000	1.00	0.00
ILE71	HD11	1.00	0.000	1.00	0.00
ILE71	H	0.94	0.000	1.00	0.00

**3.71.6 Detailed Probabilities of ILE71N:**

Overall probability: 1.000

Overall confidence: 0.917

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER70	1.00	0.80
ILE71	1.00	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	0.000	1.00	0.00
SER70	HB2	1.00	0.000	1.00	0.00
SER70	HB3	1.00	0.000	1.00	0.00
SER70	H	1.00	0.000	1.00	0.00
ILE71	HA	1.00	0.000	1.00	0.00
ILE71	HB	1.00	0.000	1.00	0.00
ILE71	HG12	1.00	0.000	1.00	0.00
ILE71	HG13	1.00	0.000	1.00	0.00
ILE71	HG21	1.00	0.000	1.00	0.00
ILE71	H	1.00	0.000	1.00	0.00
ILE71	HD11	0.94	0.000	1.00	0.00
THR72	H	1.00	0.000	1.00	0.00

**3.71.7 Detailed Probabilities of ILE71HA:**

Overall probability: 0.800

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER70	0.00	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	0.070	0.00	0.00
ILE71	HA	1.00	0.000	1.00	0.00
ILE71	HB	1.00	0.000	1.00	0.00
ILE71	HG12	1.00	0.000	1.00	0.00
ILE71	HG13	1.00	0.000	1.00	0.00
ILE71	HG21	1.00	0.000	1.00	0.00
ILE71	HD11	0.97	0.000	1.00	0.00
ILE71	H	1.00	0.000	1.00	0.00
THR72	HA	1.00	0.326	0.00	0.00
THR72	H	1.00	0.000	1.00	0.00

**3.71.8 Detailed Probabilities of ILE71HB:**

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
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	0.000	1.00	0.00
ILE71	HB	1.00	0.000	1.00	0.00
ILE71	HG12	1.00	0.000	1.00	0.00
ILE71	HG13	1.00	0.000	1.00	0.00
ILE71	HG21	1.00	0.000	1.00	0.00
ILE71	HD11	1.00	0.000	1.00	0.00
ILE71	H	1.00	0.000	1.00	0.00
THR72	H	1.00	0.000	1.00	0.00

## 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	0.000	1.00	0.00
ILE71	HB	1.00	0.000	1.00	0.00
ILE71	HG12	1.00	0.000	1.00	0.00
ILE71	HG13	1.00	0.000	1.00	0.00
ILE71	HG21	1.00	0.000	1.00	0.00
ILE71	HD11	1.00	0.000	1.00	0.00
ILE71	H	1.00	0.000	1.00	0.00
THR72	H	0.98	0.000	1.00	0.00

## 3.71.10 Detailed Probabilities of ILE71HG13:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
ILE71	1.00	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	0.000	1.00	0.00
ILE71	HB	1.00	0.000	1.00	0.00
ILE71	HG12	1.00	0.000	1.00	0.00
ILE71	HG13	1.00	0.000	1.00	0.00
ILE71	HG21	1.00	0.000	1.00	0.00
ILE71	HD11	1.00	0.000	1.00	0.00
ILE71	H	1.00	0.000	1.00	0.00

**3.71.11 Detailed Probabilities of ILE71HG21:**

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
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	0.000	1.00	0.00
ILE71	HB	1.00	0.000	1.00	0.00
ILE71	HG12	1.00	0.000	1.00	0.00
ILE71	HG13	1.00	0.000	1.00	0.00
ILE71	HG21	1.00	0.000	1.00	0.00
ILE71	HD11	0.99	0.000	1.00	0.00
ILE71	H	1.00	0.000	1.00	0.00
THR72	H	0.99	0.000	1.00	0.00
THR72	HA	0.64	0.003	1.00	0.00

**3.71.12 Detailed Probabilities of ILE71HD11:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE71	1.00	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	0.000	1.00	0.00
ILE71	HB	1.00	0.000	1.00	0.00
ILE71	HG12	1.00	0.000	1.00	0.00
ILE71	HG13	1.00	0.000	1.00	0.00
ILE71	HG21	0.99	0.000	1.00	0.00
ILE71	HD11	1.00	0.000	1.00	0.00
ILE71	H	0.94	0.000	1.00	0.00

**3.71.13 Detailed Probabilities of ILE71H:**

Overall probability: 1.000

Overall confidence: 0.917

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER70	1.00	0.80
ILE71	1.00	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	0.000	1.00	0.00
SER70	HB2	1.00	0.000	1.00	0.00
SER70	HB3	1.00	0.000	1.00	0.00
SER70	H	1.00	0.000	1.00	0.00
ILE71	HA	1.00	0.000	1.00	0.00
ILE71	HB	1.00	0.000	1.00	0.00
ILE71	HG12	1.00	0.000	1.00	0.00
ILE71	HG13	1.00	0.000	1.00	0.00
ILE71	HG21	1.00	0.000	1.00	0.00
ILE71	H	1.00	0.000	1.00	0.00
ILE71	HD11	0.94	0.000	1.00	0.00
THR72	H	1.00	0.000	1.00	0.00

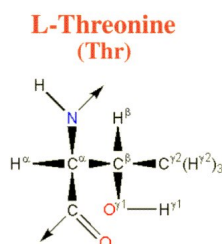


Figure 62: Image from the BMRB

Residue probability: 0.893  
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	0.778	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	0.909	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	1.000	0.833
H 3.72.8	10.252	8.272	1.597	0.911	0.909
HG1	NA	—	—	0.000	0.000

**3.72.1 Detailed Probabilities of THR72CA:**

Overall probability: 0.778  
Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE71	0.50	1.00
THR72	1.00	0.80
VAL73	0.67	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	0.326	0.00	0.00
ILE71	HG21	0.65	0.003	1.00	0.00
THR72	HA	1.00	0.000	1.00	0.00
THR72	HB	1.00	0.000	1.00	0.00
THR72	HG21	1.00	0.000	1.00	0.00
THR72	H	1.00	0.000	1.00	0.00
VAL73	HA	1.00	0.123	0.00	0.00
VAL73	H	1.00	0.000	1.00	0.00
VAL73	HG21	0.55	0.001	1.00	0.00

**3.72.2 Detailed Probabilities of THR72CB:**

Overall probability: 0.800

Overall confidence: 0.833

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR72	1.00	0.80
VAL73	0.00	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	0.000	1.00	0.00
THR72	HB	1.00	0.000	1.00	0.00
THR72	HG21	1.00	0.000	1.00	0.00
THR72	H	1.00	0.000	1.00	0.00
VAL73	H	1.00	0.174	0.00	0.00

**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	0.000	1.00	0.00
THR72	HB	1.00	0.000	1.00	0.00
THR72	HG21	1.00	0.000	1.00	0.00
THR72	H	1.00	0.000	1.00	0.00
VAL73	H	0.97	0.000	1.00	0.00

**3.72.4 Detailed Probabilities of THR72N:**

Overall probability: 0.909

Overall confidence: 0.909

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE71	1.00	1.00
THR72	1.00	0.80
VAL73	0.00	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	0.000	1.00	0.00
ILE71	HB	1.00	0.000	1.00	0.00
ILE71	HG12	0.98	0.000	1.00	0.00
ILE71	HG21	0.99	0.000	1.00	0.00
ILE71	H	1.00	0.000	1.00	0.00
ILE71	HG13	0.95	0.000	1.00	0.00
THR72	HA	1.00	0.000	1.00	0.00
THR72	HB	1.00	0.000	1.00	0.00
THR72	HG21	1.00	0.000	1.00	0.00
THR72	H	1.00	0.000	1.00	0.00
VAL73	H	1.00	0.050	0.00	0.00

## 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	0.048	0.00	0.00
ILE71	HG21	0.65	0.030	1.00	0.00
THR72	HA	1.00	0.000	1.00	0.00
THR72	HB	1.00	0.000	1.00	0.00
THR72	HG21	1.00	0.000	1.00	0.00
THR72	H	1.00	0.000	1.00	0.00
VAL73	HA	1.00	0.874	0.00	0.00
VAL73	H	1.00	0.000	1.00	0.00

## 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	0.000	1.00	0.00
THR72	HB	1.00	0.000	1.00	0.00
THR72	HG21	1.00	0.000	1.00	0.00
THR72	H	1.00	0.000	1.00	0.00
VAL73	H	1.00	0.000	1.00	0.00

**3.72.7 Detailed Probabilities of THR72HG21:**

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	0.000	1.00	0.00
THR72	HB	1.00	0.000	1.00	0.00
THR72	HG21	1.00	0.000	1.00	0.00
THR72	H	1.00	0.000	1.00	0.00
VAL73	H	0.97	0.000	1.00	0.00

**3.72.8 Detailed Probabilities of THR72H:**

Overall probability: 0.911

Overall confidence: 0.909

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE71	0.84	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	0.000	1.00	0.00
ILE71	HB	1.00	0.000	1.00	0.00
ILE71	HG12	0.98	1.061	0.02	0.00
ILE71	HG21	0.99	0.000	1.00	0.00
ILE71	H	1.00	0.000	1.00	0.00
ILE71	HG13	0.95	0.000	1.00	0.00
THR72	HA	1.00	0.000	1.00	0.00
THR72	HB	1.00	0.000	1.00	0.00
THR72	HG21	1.00	0.000	1.00	0.00
THR72	H	1.00	0.000	1.00	0.00
VAL73	H	1.00	0.000	1.00	0.00

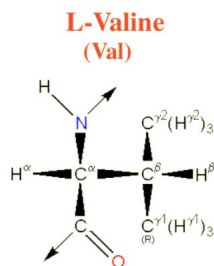
**3.73 VAL(73)**

Figure 63: Image from the BMRB

Residue probability: 0.933

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	0.750	1.000
CB 3.73.2	34.387	32.918	4.591	1.000	1.000
CG1 3.73.3	22.601	21.563	2.746	1.000	1.000
CG2 3.73.4	22.053	21.368	2.801	1.000	1.000
N 3.73.5	129.570	121.057	5.832	1.000	0.909
HA 3.73.6	4.719	4.178	0.599	0.778	1.000
HB 3.73.7	2.313	1.980	0.322	1.000	1.000
HG1 3.73.8	1.156	0.816	0.264	1.000	1.000
HG2 3.73.9	0.944	0.803	0.504	1.000	1.000
H 3.73.10	9.241	8.311	0.669	0.800	0.909

**3.73.1 Detailed Probabilities of VAL73CA:**

Overall probability: 0.750

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR72	0.00	1.00
VAL73	1.00	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	0.874	0.00	0.00
VAL73	HA	1.00	0.000	1.00	0.00
VAL73	HB	1.00	0.000	1.00	0.00
VAL73	HG11	1.00	0.000	1.00	0.00
VAL73	HG21	1.00	0.000	1.00	0.00
VAL73	H	1.00	0.000	1.00	0.00
THR74	HA	1.00	1.120	0.00	0.00
THR74	H	1.00	0.000	1.00	0.00

**3.73.2 Detailed Probabilities of VAL73CB:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL73	1.00	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	0.000	1.00	0.00
VAL73	HB	1.00	0.000	1.00	0.00
VAL73	HG11	1.00	0.000	1.00	0.00
VAL73	HG21	1.00	0.000	1.00	0.00
VAL73	H	1.00	0.000	1.00	0.00
THR74	H	1.00	0.000	1.00	0.00

**3.73.3 Detailed Probabilities of VAL73CG1:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL73	1.00	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	0.000	1.00	0.00
VAL73	HB	1.00	0.000	1.00	0.00
VAL73	HG11	1.00	0.000	1.00	0.00
VAL73	HG21	1.00	0.000	1.00	0.00
VAL73	H	1.00	0.000	1.00	0.00
THR74	H	0.97	0.000	1.00	0.00
THR74	HA	0.52	0.011	1.00	0.00

**3.73.4 Detailed Probabilities of VAL73CG2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL73	1.00	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	0.000	1.00	0.00
VAL73	HB	1.00	0.000	1.00	0.00
VAL73	HG11	1.00	0.000	1.00	0.00
VAL73	HG21	1.00	0.000	1.00	0.00
VAL73	H	1.00	0.000	1.00	0.00

**3.73.5 Detailed Probabilities of VAL73N:**

Overall probability: 1.000

Overall confidence: 0.909

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR72	1.00	0.80
VAL73	1.00	1.00
THR74	1.00	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	0.000	1.00	0.00
THR72	HB	1.00	0.000	1.00	0.00
THR72	HG21	0.98	0.000	1.00	0.00
THR72	H	1.00	0.000	1.00	0.00
VAL73	HA	1.00	0.000	1.00	0.00
VAL73	HB	1.00	0.000	1.00	0.00
VAL73	HG11	1.00	0.000	1.00	0.00
VAL73	HG21	1.00	0.000	1.00	0.00
VAL73	H	1.00	0.000	1.00	0.00
THR74	H	1.00	0.000	1.00	0.00

**3.73.6 Detailed Probabilities of VAL73HA:**

Overall probability: 0.778

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR72	0.00	1.00
VAL73	1.00	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	0.123	0.00	0.00
VAL73	HA	1.00	0.000	1.00	0.00
VAL73	HB	1.00	0.000	1.00	0.00
VAL73	HG11	1.00	0.000	1.00	0.00
VAL73	HG21	1.00	0.000	1.00	0.00
VAL73	H	1.00	0.000	1.00	0.00
THR74	HA	1.00	0.613	0.00	0.00
THR74	H	1.00	0.000	1.00	0.00
THR74	HB	0.53	0.018	1.00	0.00

**3.73.7 Detailed Probabilities of VAL73HB:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL73	1.00	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	0.000	1.00	0.00
VAL73	HB	1.00	0.000	1.00	0.00
VAL73	HG11	1.00	0.000	1.00	0.00
VAL73	HG21	1.00	0.000	1.00	0.00
VAL73	H	1.00	0.000	1.00	0.00
THR74	H	1.00	0.000	1.00	0.00

**3.73.8 Detailed Probabilities of VAL73HG11:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL73	1.00	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	0.000	1.00	0.00
VAL73	HB	1.00	0.000	1.00	0.00
VAL73	HG11	1.00	0.000	1.00	0.00
VAL73	HG21	1.00	0.000	1.00	0.00
VAL73	H	1.00	0.000	1.00	0.00
THR74	H	0.97	0.000	1.00	0.00

**3.73.9 Detailed Probabilities of VAL73HG21:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL73	1.00	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	0.000	1.00	0.00
VAL73	HB	1.00	0.000	1.00	0.00
VAL73	HG11	1.00	0.000	1.00	0.00
VAL73	HG21	1.00	0.000	1.00	0.00
VAL73	H	1.00	0.000	1.00	0.00

**3.73.10 Detailed Probabilities of VAL73H:**

Overall probability: 0.800

Overall confidence: 0.909

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR72	0.50	0.80
VAL73	1.00	1.00
THR74	1.00	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	0.000	1.00	0.00
THR72	HB	1.00	0.174	0.00	0.00
THR72	HG21	0.98	0.000	1.00	0.00
THR72	H	1.00	0.050	0.00	0.00
VAL73	HA	1.00	0.000	1.00	0.00
VAL73	HB	1.00	0.000	1.00	0.00
VAL73	HG11	1.00	0.000	1.00	0.00
VAL73	HG21	1.00	0.000	1.00	0.00
VAL73	H	1.00	0.000	1.00	0.00
THR74	H	1.00	0.000	1.00	0.00

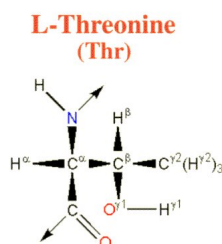


Figure 64: Image from the BMRB

Residue probability: 0.908  
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	0.800	0.833
CG2 3.74.3	20.556	21.588	1.595	1.000	0.833
N 3.74.4	124.393	115.370	5.913	1.000	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	1.000	0.833
HG2 3.74.7	1.198	1.134	0.349	1.000	0.833
H 3.74.8	8.774	8.272	1.597	1.000	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	0.613	0.00	0.00
THR74	HA	1.00	0.000	1.00	0.00
THR74	HB	1.00	0.000	1.00	0.00
THR74	HG21	1.00	0.000	1.00	0.00
THR74	H	1.00	0.000	1.00	0.00
LYS75	HA	1.00	0.540	0.00	0.00
LYS75	H	1.00	0.000	1.00	0.00

**3.74.2 Detailed Probabilities of THR74CB:**

Overall probability: 0.800

Overall confidence: 0.833

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR74	1.00	0.80
LYS75	0.00	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	0.000	1.00	0.00
THR74	HB	1.00	0.000	1.00	0.00
THR74	HG21	1.00	0.000	1.00	0.00
THR74	H	1.00	0.000	1.00	0.00
LYS75	H	1.00	0.167	0.00	0.00

**3.74.3 Detailed Probabilities of THR74CG2:**

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
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	0.000	1.00	0.00
THR74	HB	1.00	0.000	1.00	0.00
THR74	HG21	1.00	0.000	1.00	0.00
THR74	H	1.00	0.000	1.00	0.00
LYS75	H	0.95	0.000	1.00	0.00

**3.74.4 Detailed Probabilities of THR74N:**

Overall probability: 1.000

Overall confidence: 0.900

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL73	1.00	1.00
THR74	1.00	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	0.000	1.00	0.00
VAL73	HB	1.00	0.000	1.00	0.00
VAL73	HG11	0.97	0.000	1.00	0.00
VAL73	H	1.00	0.000	1.00	0.00
VAL73	HG21	0.94	0.000	1.00	0.00
THR74	HA	1.00	0.000	1.00	0.00
THR74	HB	1.00	0.000	1.00	0.00
THR74	HG21	1.00	0.000	1.00	0.00
THR74	H	1.00	0.000	1.00	0.00
LYS75	H	1.00	0.000	1.00	0.00

**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	1.120	0.00	0.00
VAL73	HG11	0.54	0.011	1.00	0.00
THR74	HA	1.00	0.000	1.00	0.00
THR74	HB	1.00	0.000	1.00	0.00
THR74	HG21	1.00	0.000	1.00	0.00
THR74	H	1.00	0.000	1.00	0.00
LYS75	HA	1.00	0.540	0.00	0.00
LYS75	H	1.00	0.000	1.00	0.00

**3.74.6 Detailed Probabilities of THR74HB:**

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	0.000	1.00	0.00
THR74	HB	1.00	0.000	1.00	0.00
THR74	HG21	1.00	0.000	1.00	0.00
THR74	H	1.00	0.000	1.00	0.00
LYS75	H	1.00	0.000	1.00	0.00

**3.74.7 Detailed Probabilities of THR74HG21:**

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
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	0.000	1.00	0.00
THR74	HB	1.00	0.000	1.00	0.00
THR74	HG21	1.00	0.000	1.00	0.00
THR74	H	1.00	0.000	1.00	0.00
LYS75	H	0.95	0.000	1.00	0.00

**3.74.8 Detailed Probabilities of THR74H:**

Overall probability: 1.000

Overall confidence: 0.900

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL73	1.00	1.00
THR74	1.00	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	0.000	1.00	0.00
VAL73	HB	1.00	0.000	1.00	0.00
VAL73	HG11	0.97	0.000	1.00	0.00
VAL73	H	1.00	0.000	1.00	0.00
VAL73	HG21	0.94	0.000	1.00	0.00
THR74	HA	1.00	0.000	1.00	0.00
THR74	HB	1.00	0.000	1.00	0.00
THR74	HG21	1.00	0.000	1.00	0.00
THR74	H	1.00	0.000	1.00	0.00
LYS75	H	1.00	0.000	1.00	0.00

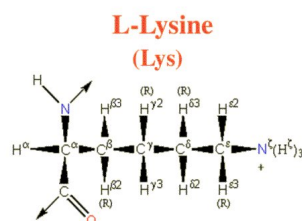


Figure 65: Image from the BMRB

Residue probability: 0.885  
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	0.800	1.000
CB 3.75.2	34.954	32.981	3.186	0.803	1.000
CG 3.75.3	22.886	24.941	1.956	0.900	0.909
CD 3.75.4	28.780	29.020	2.193	0.878	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	0.704	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	1.000	1.000
HG 3.75.10	1.010	1.358	0.344	1.000	0.909
HD2 3.75.11	-0.917	1.614	0.957	1.000	0.889
HD3 3.75.12	0.714	1.595	0.387	1.000	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	0.575	0.875
H 3.75.15	9.472	8.185	0.605	0.900	0.909
HZ	NA	—	—	0.000	0.000

#### 3.75.1 Detailed Probabilities of LYS75CA:

Overall probability: 0.800  
Overall confidence: 1.000

#### Inter- and intra-residue probability

Residue	Probability	Confidence
THR74	0.00	1.00
LYS75	1.00	1.00
GLU76	0.50	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	0.540	0.00	0.00
LYS75	HA	1.00	0.000	1.00	0.00
LYS75	HB2	1.00	0.000	1.00	0.00
LYS75	HB3	1.00	0.000	1.00	0.00
LYS75	HG2	1.00	0.000	1.00	0.00
LYS75	HD2	0.98	0.000	1.00	0.00
LYS75	HD3	0.98	0.000	1.00	0.00
LYS75	H	1.00	0.000	1.00	0.00
GLU76	HA	1.00	0.166	0.00	0.00
GLU76	H	1.00	0.000	1.00	0.00

**3.75.2 Detailed Probabilities of LYS75CB:**

Overall probability: 0.803

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	0.000	1.00	0.00
LYS75	HB2	1.00	0.000	1.00	0.00
LYS75	HB3	1.00	0.000	1.00	0.00
LYS75	HG2	1.00	0.000	1.00	0.00
LYS75	HD2	1.00	0.000	1.00	0.00
LYS75	HD3	1.00	0.000	1.00	0.00
LYS75	HE2	0.98	0.412	0.02	0.00
LYS75	HE3	0.99	0.183	0.01	0.00
LYS75	H	1.00	0.000	1.00	0.00
GLU76	H	1.00	0.000	1.00	0.00

## 3.75.3 Detailed Probabilities of LYS75CG:

Overall probability: 0.900

Overall confidence: 0.909

## Inter- and intra-residue probability

Residue	Probability	Confidence
LYS75	0.89	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	0.000	1.00	0.00
LYS75	HB2	1.00	0.000	1.00	0.00
LYS75	HB3	1.00	0.000	1.00	0.00
LYS75	HG2	1.00	0.000	1.00	0.00
LYS75	HD2	1.00	0.000	1.00	0.00
LYS75	HD3	1.00	0.000	1.00	0.00
LYS75	HE2	1.00	0.000	1.00	0.00
LYS75	HE3	1.00	0.274	0.00	0.00
LYS75	H	1.00	0.000	1.00	0.00
GLU76	H	0.97	0.000	1.00	0.00

**3.75.4 Detailed Probabilities of LYS75CD:**

Overall probability: 0.878

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS75	0.88	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	2.949	0.02	0.00
LYS75	HB2	1.00	0.000	1.00	0.00
LYS75	HB3	1.00	0.000	1.00	0.00
LYS75	HG2	1.00	0.000	1.00	0.00
LYS75	HD2	1.00	0.000	1.00	0.00
LYS75	HD3	1.00	0.000	1.00	0.00
LYS75	HE2	1.00	0.000	1.00	0.00
LYS75	HE3	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
LYS75	HB3	0.99	0.000	1.00	0.00
LYS75	HG2	1.00	0.000	1.00	0.00
LYS75	HD2	1.00	0.000	1.00	0.00
LYS75	HD3	1.00	0.000	1.00	0.00
LYS75	HE2	1.00	0.000	1.00	0.00
LYS75	HE3	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
THR74	HB	1.00	0.000	1.00	0.00
THR74	HG21	0.96	0.000	1.00	0.00
THR74	H	1.00	0.000	1.00	0.00
LYS75	HA	1.00	0.000	1.00	0.00
LYS75	HB2	1.00	0.000	1.00	0.00
LYS75	HB3	1.00	0.000	1.00	0.00
LYS75	HG2	1.00	0.000	1.00	0.00
LYS75	H	1.00	0.000	1.00	0.00
LYS75	HD2	0.88	0.000	1.00	0.00
LYS75	HD3	0.87	0.000	1.00	0.00
GLU76	H	1.00	0.000	1.00	0.00

**3.75.7 Detailed Probabilities of LYS75HA:**

Overall probability: 0.704

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR74	0.00	1.00
LYS75	0.72	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	0.540	0.00	0.00
LYS75	HA	1.00	0.000	1.00	0.00
LYS75	HB2	1.00	0.000	1.00	0.00
LYS75	HB3	1.00	0.000	1.00	0.00
LYS75	HG2	1.00	0.000	1.00	0.00
LYS75	HD2	0.98	2.949	0.02	0.00
LYS75	HD3	0.98	2.949	0.02	0.00
LYS75	H	1.00	0.000	1.00	0.00
GLU76	HA	1.00	0.004	1.00	0.00
GLU76	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
LYS75	HB2	1.00	0.000	1.00	0.00
LYS75	HB3	1.00	0.000	1.00	0.00
LYS75	HG2	1.00	0.000	1.00	0.00
LYS75	HD2	1.00	0.000	1.00	0.00
LYS75	HD3	1.00	0.000	1.00	0.00
LYS75	HE2	0.98	0.000	1.00	0.00
LYS75	HE3	0.99	0.000	1.00	0.00
LYS75	H	1.00	0.000	1.00	0.00
GLU76	H	1.00	0.000	1.00	0.00

**3.75.9 Detailed Probabilities of LYS75HB3:**

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
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	0.000	1.00	0.00
LYS75	HB2	1.00	0.000	1.00	0.00
LYS75	HB3	1.00	0.000	1.00	0.00
LYS75	HG2	1.00	0.000	1.00	0.00
LYS75	HD2	1.00	0.000	1.00	0.00
LYS75	HD3	1.00	0.000	1.00	0.00
LYS75	HE2	0.99	0.000	1.00	0.00
LYS75	HE3	0.99	0.000	1.00	0.00
LYS75	H	1.00	0.000	1.00	0.00
GLU76	H	1.00	0.000	1.00	0.00

## 3.75.10 Detailed Probabilities of LYS75HG2:

Overall probability: 1.000

Overall confidence: 0.909

## Inter- and intra-residue probability

Residue	Probability	Confidence
LYS75	1.00	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	0.000	1.00	0.00
LYS75	HB2	1.00	0.000	1.00	0.00
LYS75	HB3	1.00	0.000	1.00	0.00
LYS75	HG2	1.00	0.000	1.00	0.00
LYS75	HD2	1.00	0.000	1.00	0.00
LYS75	HD3	1.00	0.000	1.00	0.00
LYS75	HE2	1.00	0.000	1.00	0.00
LYS75	HE3	1.00	0.000	1.00	0.00
LYS75	H	1.00	0.000	1.00	0.00
GLU76	H	0.97	0.000	1.00	0.00

**3.75.11 Detailed Probabilities of LYS75HD2:**

Overall probability: 1.000

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS75	1.00	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	0.000	1.00	0.00
LYS75	HB2	1.00	0.000	1.00	0.00
LYS75	HB3	1.00	0.000	1.00	0.00
LYS75	HG2	1.00	0.000	1.00	0.00
LYS75	HD2	1.00	0.000	1.00	0.00
LYS75	HD3	1.00	0.000	1.00	0.00
LYS75	HE2	1.00	0.000	1.00	0.00
LYS75	HE3	1.00	0.000	1.00	0.00
LYS75	H	0.88	0.000	1.00	0.00

**3.75.12 Detailed Probabilities of LYS75HD3:**

Overall probability: 1.000

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS75	1.00	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	0.000	1.00	0.00
LYS75	HB2	1.00	0.000	1.00	0.00
LYS75	HB3	1.00	0.000	1.00	0.00
LYS75	HG2	1.00	0.000	1.00	0.00
LYS75	HD2	1.00	0.000	1.00	0.00
LYS75	HD3	1.00	0.000	1.00	0.00
LYS75	HE2	1.00	0.000	1.00	0.00
LYS75	HE3	1.00	0.000	1.00	0.00
LYS75	H	0.87	0.000	1.00	0.00

**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	0.412	0.02	0.00
LYS75	HB3	0.99	0.817	0.01	0.00
LYS75	HG2	1.00	0.000	1.00	0.00
LYS75	HD2	1.00	0.000	1.00	0.00
LYS75	HD3	1.00	0.000	1.00	0.00
LYS75	HE2	1.00	0.000	1.00	0.00
LYS75	HE3	1.00	0.000	1.00	0.00

**3.75.14 Detailed Probabilities of LYS75HE3:**

Overall probability: 0.575

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS75	0.57	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	0.183	0.01	0.00
LYS75	HB3	0.99	0.543	0.01	0.00
LYS75	HG2	1.00	0.274	0.00	0.00
LYS75	HD2	1.00	0.000	1.00	0.00
LYS75	HD3	1.00	0.000	1.00	0.00
LYS75	HE2	1.00	0.000	1.00	0.00
LYS75	HE3	1.00	0.000	1.00	0.00

**3.75.15 Detailed Probabilities of LYS75H:**

Overall probability: 0.900

Overall confidence: 0.909

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR74	0.75	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	0.000	1.00	0.00
THR74	HB	1.00	0.167	0.00	0.00
THR74	HG21	0.96	0.000	1.00	0.00
THR74	H	1.00	0.000	1.00	0.00
LYS75	HA	1.00	0.000	1.00	0.00
LYS75	HB2	1.00	0.000	1.00	0.00
LYS75	HB3	1.00	0.000	1.00	0.00
LYS75	HG2	1.00	0.000	1.00	0.00
LYS75	H	1.00	0.000	1.00	0.00
GLU76	H	1.00	0.000	1.00	0.00

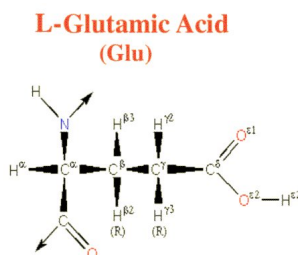


Figure 66: Image from the BMRB

Residue probability: 0.967  
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	1.000	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	1.000	1.000
HA 3.76.5	3.779	4.245	0.429	0.778	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	1.000	0.875
HG3 3.76.9	2.186	2.233	0.232	1.000	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	0.004	1.00	0.00
GLU76	HA	1.00	0.000	1.00	0.00
GLU76	HB2	1.00	0.000	1.00	0.00
GLU76	HB3	1.00	0.000	1.00	0.00
GLU76	HG2	1.00	0.000	1.00	0.00
GLU76	HG3	1.00	0.000	1.00	0.00
GLU76	H	1.00	0.000	1.00	0.00
ASN77	HA	1.00	0.171	0.00	0.00
ASN77	H	1.00	0.000	1.00	0.00

**3.76.2 Detailed Probabilities of GLU76CB:**

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	0.000	1.00	0.00
GLU76	HB2	1.00	0.000	1.00	0.00
GLU76	HB3	1.00	0.000	1.00	0.00
GLU76	HG2	1.00	0.000	1.00	0.00
GLU76	HG3	1.00	0.000	1.00	0.00
GLU76	H	1.00	0.000	1.00	0.00
ASN77	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
GLU76	HB2	1.00	0.000	1.00	0.00
GLU76	HB3	1.00	0.000	1.00	0.00
GLU76	HG2	1.00	0.000	1.00	0.00
GLU76	HG3	1.00	0.000	1.00	0.00
GLU76	H	1.00	0.000	1.00	0.00
ASN77	H	0.97	0.000	1.00	0.00

**3.76.4 Detailed Probabilities of GLU76N:**

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	0.000	1.00	0.00
LYS75	HB2	1.00	0.000	1.00	0.00
LYS75	HB3	1.00	0.000	1.00	0.00
LYS75	HG2	0.98	0.000	1.00	0.00
LYS75	H	1.00	0.000	1.00	0.00
LYS75	HD2	0.59	0.000	1.00	0.00
LYS75	HD3	0.62	0.000	1.00	0.00
GLU76	HA	1.00	0.000	1.00	0.00
GLU76	HB2	1.00	0.000	1.00	0.00
GLU76	HB3	1.00	0.000	1.00	0.00
GLU76	HG2	1.00	0.000	1.00	0.00
GLU76	HG3	1.00	0.000	1.00	0.00
GLU76	H	1.00	0.000	1.00	0.00
ASN77	H	1.00	0.000	1.00	0.00

## 3.76.5 Detailed Probabilities of GLU76HA:

Overall probability: 0.778

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
LYS75	0.00	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	0.166	0.00	0.00
GLU76	HA	1.00	0.000	1.00	0.00
GLU76	HB2	1.00	0.000	1.00	0.00
GLU76	HB3	1.00	0.000	1.00	0.00
GLU76	HG2	1.00	0.000	1.00	0.00
GLU76	HG3	1.00	0.000	1.00	0.00
GLU76	H	1.00	0.000	1.00	0.00
ASN77	HA	1.00	0.741	0.00	0.00
ASN77	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
GLU76	HB2	1.00	0.000	1.00	0.00
GLU76	HB3	1.00	0.000	1.00	0.00
GLU76	HG2	1.00	0.000	1.00	0.00
GLU76	HG3	1.00	0.000	1.00	0.00
GLU76	H	1.00	0.000	1.00	0.00
ASN77	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
GLU76	HB2	1.00	0.000	1.00	0.00
GLU76	HB3	1.00	0.000	1.00	0.00
GLU76	HG2	1.00	0.000	1.00	0.00
GLU76	HG3	1.00	0.000	1.00	0.00
GLU76	H	1.00	0.000	1.00	0.00
ASN77	H	1.00	0.000	1.00	0.00
ASN77	HB2	0.50	0.012	1.00	0.00

**3.76.8 Detailed Probabilities of GLU76HG2:**

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	0.000	1.00	0.00
GLU76	HB2	1.00	0.000	1.00	0.00
GLU76	HB3	1.00	0.000	1.00	0.00
GLU76	HG2	1.00	0.000	1.00	0.00
GLU76	HG3	1.00	0.000	1.00	0.00
GLU76	H	1.00	0.000	1.00	0.00
ASN77	H	0.97	0.000	1.00	0.00

**3.76.9 Detailed Probabilities of GLU76HG3:**

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
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	0.000	1.00	0.00
GLU76	HB2	1.00	0.000	1.00	0.00
GLU76	HB3	1.00	0.000	1.00	0.00
GLU76	HG2	1.00	0.000	1.00	0.00
GLU76	HG3	1.00	0.000	1.00	0.00
GLU76	H	1.00	0.000	1.00	0.00
ASN77	H	0.97	0.000	1.00	0.00

**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	0.000	1.00	0.00
LYS75	HB2	1.00	0.000	1.00	0.00
LYS75	HB3	1.00	0.000	1.00	0.00
LYS75	HG2	0.98	0.000	1.00	0.00
LYS75	H	1.00	0.000	1.00	0.00
GLU76	HA	1.00	0.000	1.00	0.00
GLU76	HB2	1.00	0.000	1.00	0.00
GLU76	HB3	1.00	0.000	1.00	0.00
GLU76	HG2	1.00	0.000	1.00	0.00
GLU76	HG3	1.00	0.000	1.00	0.00
GLU76	H	1.00	0.000	1.00	0.00
ASN77	H	1.00	0.000	1.00	0.00

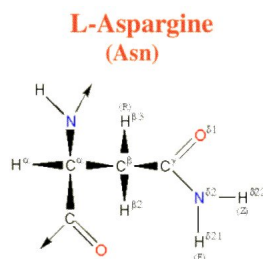


Figure 67: Image from the BMRB

Residue probability: 0.950  
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	0.750	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	0.750	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	1.000	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: 0.750  
Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU76	0.00	1.00
ASN77	1.00	1.00
GLU78	0.00	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	0.741	0.00	0.00
ASN77	HA	1.00	0.000	1.00	0.00
ASN77	HB2	1.00	0.000	1.00	0.00
ASN77	HB3	1.00	0.000	1.00	0.00
ASN77	H	1.00	0.000	1.00	0.00
ASN77	HD21	1.00	0.000	1.00	0.00
ASN77	HD22	1.00	0.000	1.00	0.00
GLU78	HA	1.00	0.660	0.00	0.00

**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	0.000	1.00	0.00
ASN77	HB2	1.00	0.000	1.00	0.00
ASN77	HB3	1.00	0.000	1.00	0.00
ASN77	H	1.00	0.000	1.00	0.00
ASN77	HD21	1.00	0.000	1.00	0.00
ASN77	HD22	1.00	0.000	1.00	0.00

**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	0.00	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	0.000	1.00	0.00
GLU76	HB2	1.00	0.000	1.00	0.00
GLU76	HB3	1.00	0.000	1.00	0.00
GLU76	HG2	0.98	0.000	1.00	0.00
GLU76	HG3	0.97	0.000	1.00	0.00
GLU76	H	1.00	0.000	1.00	0.00
ASN77	HA	1.00	0.000	1.00	0.00
ASN77	HB2	1.00	0.000	1.00	0.00
ASN77	HB3	1.00	0.000	1.00	0.00
ASN77	H	1.00	0.000	1.00	0.00
ASN77	HD21	0.98	0.004	1.00	0.00
ASN77	HD22	0.63	0.009	1.00	0.00

**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**

## 3.77 ASN(77)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN77	HA	1.00	0.000	1.00	0.00
ASN77	HB2	1.00	0.000	1.00	0.00
ASN77	HB3	1.00	0.000	1.00	0.00
ASN77	H	0.98	0.000	1.00	0.00
ASN77	HD21	1.00	0.000	1.00	0.00
ASN77	HD22	1.00	0.000	1.00	0.00

**3.77.5 Detailed Probabilities of ASN77HA:**

Overall probability: 0.750

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU76	0.00	1.00
ASN77	1.00	1.00
GLU78	0.00	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	0.171	0.00	0.00
ASN77	HA	1.00	0.000	1.00	0.00
ASN77	HB2	1.00	0.000	1.00	0.00
ASN77	HB3	1.00	0.000	1.00	0.00
ASN77	H	1.00	0.000	1.00	0.00
ASN77	HD21	1.00	0.000	1.00	0.00
ASN77	HD22	1.00	0.000	1.00	0.00
GLU78	HA	1.00	0.660	0.00	0.00

**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	0.000	1.00	0.00
ASN77	HB2	1.00	0.000	1.00	0.00
ASN77	HB3	1.00	0.000	1.00	0.00
ASN77	H	1.00	0.000	1.00	0.00
ASN77	HD21	1.00	0.000	1.00	0.00
ASN77	HD22	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ASN77	HB2	1.00	0.000	1.00	0.00
ASN77	HB3	1.00	0.000	1.00	0.00
ASN77	H	1.00	0.000	1.00	0.00
ASN77	HD21	1.00	0.000	1.00	0.00
ASN77	HD22	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
GLU76	HB2	1.00	0.000	1.00	0.00
GLU76	HB3	1.00	0.000	1.00	0.00
GLU76	HG2	0.98	0.000	1.00	0.00
GLU76	HG3	0.97	0.000	1.00	0.00
GLU76	H	1.00	0.000	1.00	0.00
ASN77	HA	1.00	0.000	1.00	0.00
ASN77	HB2	1.00	0.000	1.00	0.00
ASN77	HB3	1.00	0.000	1.00	0.00
ASN77	H	1.00	0.000	1.00	0.00
ASN77	HD21	0.98	0.000	1.00	0.00
ASN77	HD22	0.63	0.000	1.00	0.00

**3.77.9 Detailed Probabilities of ASN77HD21:**

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	0.000	1.00	0.00
ASN77	HB2	1.00	0.000	1.00	0.00
ASN77	HB3	1.00	0.000	1.00	0.00
ASN77	H	0.98	0.004	1.00	0.00
ASN77	HD21	1.00	0.000	1.00	0.00
ASN77	HD22	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ASN77	HB2	1.00	0.000	1.00	0.00
ASN77	HB3	1.00	0.000	1.00	0.00
ASN77	HD21	1.00	0.000	1.00	0.00
ASN77	HD22	1.00	0.000	1.00	0.00
ASN77	H	0.63	0.009	1.00	0.00

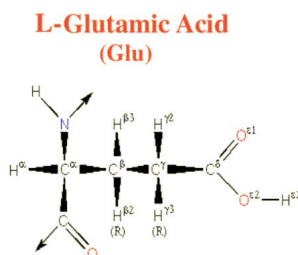


Figure 68: Image from the BMRB

Residue probability: 0.970  
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	0.889	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	1.000	0.750
N	NA	—	—	0.000	0.000
HA 3.78.4	4.022	4.245	0.429	0.875	0.889
HB2 3.78.5	2.066	2.021	0.233	1.000	0.750
HB3 3.78.6	2.067	1.994	0.244	1.000	0.750
HG2 3.78.7	2.331	2.258	0.226	1.000	0.750
HG3 3.78.8	2.328	2.233	0.232	1.000	0.750
H	NA	—	—	0.000	0.000
HE2	NA	—	—	0.000	0.000

**3.78.1 Detailed Probabilities of GLU78CA:**

Overall probability: 0.889  
Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASN77	0.50	1.00
GLU78	1.00	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	0.660	0.00	0.00
ASN77	H	0.89	0.006	1.00	0.00
GLU78	HA	1.00	0.000	1.00	0.00
GLU78	HB2	1.00	0.000	1.00	0.00
GLU78	HB3	1.00	0.000	1.00	0.00
GLU78	HG2	1.00	0.000	1.00	0.00
GLU78	HG3	1.00	0.000	1.00	0.00
GLU79	HA	1.00	0.002	1.00	0.00
GLU79	H	1.00	0.000	1.00	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	0.000	1.00	0.00
GLU78	HB2	1.00	0.000	1.00	0.00
GLU78	HB3	1.00	0.000	1.00	0.00
GLU78	HG2	1.00	0.000	1.00	0.00
GLU78	HG3	1.00	0.000	1.00	0.00
GLU79	H	1.00	0.000	1.00	0.00
GLU79	HA	0.69	0.002	1.00	0.00

**3.78.3 Detailed Probabilities of GLU78CG:**

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
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	0.000	1.00	0.00
GLU78	HB2	1.00	0.000	1.00	0.00
GLU78	HB3	1.00	0.000	1.00	0.00
GLU78	HG2	1.00	0.000	1.00	0.00
GLU78	HG3	1.00	0.000	1.00	0.00
GLU79	H	0.98	0.000	1.00	0.00

**3.78.4 Detailed Probabilities of GLU78HA:**

Overall probability: 0.875

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASN77	0.00	1.00
GLU78	1.00	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	0.660	0.00	0.00
GLU78	HA	1.00	0.000	1.00	0.00
GLU78	HB2	1.00	0.000	1.00	0.00
GLU78	HB3	1.00	0.000	1.00	0.00
GLU78	HG2	1.00	0.000	1.00	0.00
GLU78	HG3	1.00	0.000	1.00	0.00
GLU79	HA	1.00	0.004	1.00	0.00
GLU79	H	1.00	0.000	1.00	0.00

**3.78.5 Detailed Probabilities of GLU78HB2:**

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	0.000	1.00	0.00
GLU78	HB2	1.00	0.000	1.00	0.00
GLU78	HB3	1.00	0.000	1.00	0.00
GLU78	HG2	1.00	0.000	1.00	0.00
GLU78	HG3	1.00	0.000	1.00	0.00
GLU79	H	1.00	0.000	1.00	0.00

**3.78.6 Detailed Probabilities of GLU78HB3:**

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
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	0.000	1.00	0.00
GLU78	HB2	1.00	0.000	1.00	0.00
GLU78	HB3	1.00	0.000	1.00	0.00
GLU78	HG2	1.00	0.000	1.00	0.00
GLU78	HG3	1.00	0.000	1.00	0.00
GLU79	H	1.00	0.000	1.00	0.00

**3.78.7 Detailed Probabilities of GLU78HG2:**

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
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	0.000	1.00	0.00
GLU78	HB2	1.00	0.000	1.00	0.00
GLU78	HB3	1.00	0.000	1.00	0.00
GLU78	HG2	1.00	0.000	1.00	0.00
GLU78	HG3	1.00	0.000	1.00	0.00
GLU79	H	0.98	0.000	1.00	0.00

**3.78.8 Detailed Probabilities of GLU78HG3:**

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
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	0.000	1.00	0.00
GLU78	HB2	1.00	0.000	1.00	0.00
GLU78	HB3	1.00	0.000	1.00	0.00
GLU78	HG2	1.00	0.000	1.00	0.00
GLU78	HG3	1.00	0.000	1.00	0.00
GLU79	H	0.97	0.000	1.00	0.00

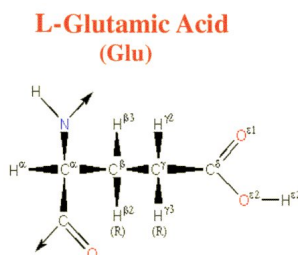
**3.79 GLU(79)**

Figure 69: Image from the BMRB

Residue probability: 0.991

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	1.000	1.000
CB 3.79.2	28.980	30.185	4.018	1.000	0.875
CG 3.79.3	36.541	36.085	1.533	1.000	0.875
N 3.79.4	117.872	120.574	4.837	1.000	0.923
HA 3.79.5	4.003	4.245	0.429	0.909	1.000
HB2 3.79.6	2.010	2.021	0.233	1.000	0.875
HB3 3.79.7	1.935	1.994	0.244	1.000	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	1.000	0.923
HE2	NA	—	—	0.000	0.000

**3.79.1 Detailed Probabilities of GLU79CA:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU78	1.00	1.00
GLU79	1.00	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	0.004	1.00	0.00
GLU79	HA	1.00	0.000	1.00	0.00
GLU79	HB2	1.00	0.000	1.00	0.00
GLU79	HB3	1.00	0.000	1.00	0.00
GLU79	HG2	1.00	0.000	1.00	0.00
GLU79	HG3	1.00	0.000	1.00	0.00
GLU79	H	1.00	0.000	1.00	0.00
LEU80	HA	1.00	0.012	1.00	0.00
LEU80	H	1.00	0.000	1.00	0.00

**3.79.2 Detailed Probabilities of GLU79CB:**

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
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	0.000	1.00	0.00
GLU79	HB2	1.00	0.000	1.00	0.00
GLU79	HB3	1.00	0.000	1.00	0.00
GLU79	HG2	1.00	0.000	1.00	0.00
GLU79	HG3	1.00	0.000	1.00	0.00
GLU79	H	1.00	0.000	1.00	0.00
LEU80	H	1.00	0.000	1.00	0.00

**3.79.3 Detailed Probabilities of GLU79CG:**

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	0.00
GLU79	HB2	1.00	0.000	1.00	0.00
GLU79	HB3	1.00	0.000	1.00	0.00
GLU79	HG2	1.00	0.000	1.00	0.00
GLU79	HG3	1.00	0.000	1.00	0.00
GLU79	H	1.00	0.000	1.00	0.00
LEU80	H	0.97	0.000	1.00	0.00

**3.79.4 Detailed Probabilities of GLU79N:**

Overall probability: 1.000

Overall confidence: 0.923

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU78	1.00	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	0.000	1.00	0.00
GLU78	HB2	1.00	0.000	1.00	0.00
GLU78	HB3	1.00	0.000	1.00	0.00
GLU78	HG2	0.98	0.000	1.00	0.00
GLU78	HG3	0.97	0.000	1.00	0.00
GLU79	HA	1.00	0.000	1.00	0.00
GLU79	HB2	1.00	0.000	1.00	0.00
GLU79	HB3	1.00	0.000	1.00	0.00
GLU79	HG2	1.00	0.000	1.00	0.00
GLU79	HG3	1.00	0.000	1.00	0.00
GLU79	H	1.00	0.000	1.00	0.00
LEU80	H	1.00	0.000	1.00	0.00
LEU80	HA	0.93	0.003	1.00	0.00
LEU80	HB2	0.69	0.005	1.00	0.00

## 3.79.5 Detailed Probabilities of GLU79HA:

Overall probability: 0.909

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
GLU78	1.00	1.00
GLU79	1.00	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	0.002	1.00	0.00
GLU78	HB2	0.69	0.002	1.00	0.00
GLU78	HB3	0.81	0.002	1.00	0.00
GLU79	HA	1.00	0.000	1.00	0.00
GLU79	HB2	1.00	0.000	1.00	0.00
GLU79	HB3	1.00	0.000	1.00	0.00
GLU79	HG2	1.00	0.000	1.00	0.00
GLU79	HG3	1.00	0.000	1.00	0.00
GLU79	H	1.00	0.000	1.00	0.00
LEU80	HA	1.00	0.202	0.00	0.00
LEU80	H	1.00	0.000	1.00	0.00

**3.79.6 Detailed Probabilities of GLU79HB2:**

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
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	0.000	1.00	0.00
GLU79	HB2	1.00	0.000	1.00	0.00
GLU79	HB3	1.00	0.000	1.00	0.00
GLU79	HG2	1.00	0.000	1.00	0.00
GLU79	HG3	1.00	0.000	1.00	0.00
GLU79	H	1.00	0.000	1.00	0.00
LEU80	H	1.00	0.000	1.00	0.00

**3.79.7 Detailed Probabilities of GLU79HB3:**

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
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	0.000	1.00	0.00
GLU79	HB2	1.00	0.000	1.00	0.00
GLU79	HB3	1.00	0.000	1.00	0.00
GLU79	HG2	1.00	0.000	1.00	0.00
GLU79	HG3	1.00	0.000	1.00	0.00
GLU79	H	1.00	0.000	1.00	0.00
LEU80	H	1.00	0.000	1.00	0.00

**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	0.00
GLU79	HB2	1.00	0.000	1.00	0.00
GLU79	HB3	1.00	0.000	1.00	0.00
GLU79	HG2	1.00	0.000	1.00	0.00
GLU79	HG3	1.00	0.000	1.00	0.00
GLU79	H	1.00	0.000	1.00	0.00
LEU80	H	0.97	0.000	1.00	0.00

**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	0.00
GLU79	HB2	1.00	0.000	1.00	0.00
GLU79	HB3	1.00	0.000	1.00	0.00
GLU79	HG2	1.00	0.000	1.00	0.00
GLU79	HG3	1.00	0.000	1.00	0.00
GLU79	H	1.00	0.000	1.00	0.00
LEU80	H	0.97	0.000	1.00	0.00

**3.79.10 Detailed Probabilities of GLU79H:**

Overall probability: 1.000

Overall confidence: 0.923

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU78	1.00	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	0.000	1.00	0.00
GLU78	HB2	1.00	0.000	1.00	0.00
GLU78	HB3	1.00	0.000	1.00	0.00
GLU78	HG2	0.98	0.000	1.00	0.00
GLU78	HG3	0.97	0.000	1.00	0.00
GLU79	HA	1.00	0.000	1.00	0.00
GLU79	HB2	1.00	0.000	1.00	0.00
GLU79	HB3	1.00	0.000	1.00	0.00
GLU79	HG2	1.00	0.000	1.00	0.00
GLU79	HG3	1.00	0.000	1.00	0.00
GLU79	H	1.00	0.000	1.00	0.00
LEU80	H	1.00	0.000	1.00	0.00
LEU80	HB2	0.69	0.010	1.00	0.00

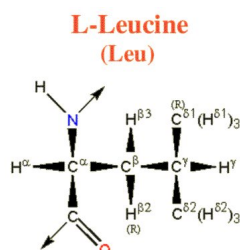
**3.80 LEU(80)**

Figure 70: Image from the BMRB

Residue probability: 0.985

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	0.800	1.000
CB 3.80.2	42.541	42.389	3.750	1.000	1.000
CG 3.80.3	26.770	26.892	3.086	1.000	1.000
CD1 3.80.4	25.912	24.837	3.657	1.000	1.000
CD2 3.80.5	24.730	24.201	3.117	1.000	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	1.000	1.000
HB2 3.80.8	1.418	1.601	0.373	1.000	1.000
HB3 3.80.9	1.295	1.508	0.398	1.000	1.000
HG 3.80.10	1.505	1.510	0.340	1.000	1.000
HD1 3.80.11	0.953	0.739	0.294	1.000	1.000
HD2 3.80.12	0.876	0.727	0.421	1.000	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: 0.800

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU79	0.00	1.00
LEU80	1.00	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	0.202	0.00	0.00
LEU80	HA	1.00	0.000	1.00	0.00
LEU80	HB2	1.00	0.000	1.00	0.00
LEU80	HB3	1.00	0.000	1.00	0.00
LEU80	HG	1.00	0.000	1.00	0.00
LEU80	HD11	0.99	0.000	1.00	0.00
LEU80	HD21	0.99	0.000	1.00	0.00
LEU80	H	1.00	0.000	1.00	0.00
ASP81	HA	1.00	0.362	0.00	0.00
ASP81	H	1.00	0.000	1.00	0.00

**3.80.2 Detailed Probabilities of LEU80CB:**

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

**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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU80	HA	1.00	0.000	1.00	0.00
LEU80	HB2	1.00	0.000	1.00	0.00
LEU80	HB3	1.00	0.000	1.00	0.00
LEU80	HG	1.00	0.000	1.00	0.00
LEU80	HD11	1.00	0.000	1.00	0.00
LEU80	HD21	1.00	0.000	1.00	0.00
LEU80	H	1.00	0.000	1.00	0.00
ASP81	H	1.00	0.000	1.00	0.00

## 3.80.3 Detailed Probabilities of LEU80CG:

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

## 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	0.000	1.00	0.00
LEU80	HB2	1.00	0.000	1.00	0.00
LEU80	HB3	1.00	0.000	1.00	0.00
LEU80	HG	1.00	0.000	1.00	0.00
LEU80	HD11	1.00	0.000	1.00	0.00
LEU80	HD21	1.00	0.000	1.00	0.00
LEU80	H	1.00	0.000	1.00	0.00
ASP81	H	0.97	0.000	1.00	0.00

## 3.80.4 Detailed Probabilities of LEU80CD1:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
LEU80	1.00	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	0.000	1.00	0.00
LEU80	HB2	1.00	0.000	1.00	0.00
LEU80	HB3	1.00	0.000	1.00	0.00
LEU80	HG	1.00	0.000	1.00	0.00
LEU80	HD11	1.00	0.000	1.00	0.00
LEU80	HD21	1.00	0.000	1.00	0.00
LEU80	H	0.86	0.000	1.00	0.00

**3.80.5 Detailed Probabilities of LEU80CD2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU80	1.00	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	0.00
LEU80	HB2	1.00	0.000	1.00	0.00
LEU80	HB3	1.00	0.000	1.00	0.00
LEU80	HG	1.00	0.000	1.00	0.00
LEU80	HD11	1.00	0.000	1.00	0.00
LEU80	HD21	1.00	0.000	1.00	0.00
LEU80	H	0.85	0.000	1.00	0.00

**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	0.000	1.00	0.00
GLU79	HB2	1.00	0.000	1.00	0.00
GLU79	HB3	1.00	0.000	1.00	0.00
GLU79	HG2	0.98	0.000	1.00	0.00
GLU79	HG3	0.97	0.000	1.00	0.00
GLU79	H	1.00	0.000	1.00	0.00
LEU80	HA	1.00	0.000	1.00	0.00
LEU80	HB2	1.00	0.000	1.00	0.00
LEU80	HB3	1.00	0.000	1.00	0.00
LEU80	HG	1.00	0.000	1.00	0.00
LEU80	H	1.00	0.000	1.00	0.00
LEU80	HD11	0.88	0.000	1.00	0.00
LEU80	HD21	0.87	0.000	1.00	0.00
ASP81	H	1.00	0.000	1.00	0.00

**3.80.7 Detailed Probabilities of LEU80HA:**

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
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	0.012	1.00	0.00
GLU79	H	0.93	0.003	1.00	0.00
LEU80	HA	1.00	0.000	1.00	0.00
LEU80	HB2	1.00	0.000	1.00	0.00
LEU80	HB3	1.00	0.000	1.00	0.00
LEU80	HG	1.00	0.000	1.00	0.00
LEU80	HD11	0.99	0.000	1.00	0.00
LEU80	HD21	0.99	0.000	1.00	0.00
LEU80	H	1.00	0.000	1.00	0.00
ASP81	HA	1.00	0.026	1.00	0.00
ASP81	H	1.00	0.000	1.00	0.00

**3.80.8 Detailed Probabilities of LEU80HB2:**

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

**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	0.000	1.00	0.00
LEU80	HB2	1.00	0.000	1.00	0.00
LEU80	HB3	1.00	0.000	1.00	0.00
LEU80	HG	1.00	0.000	1.00	0.00
LEU80	HD11	1.00	0.000	1.00	0.00
LEU80	HD21	1.00	0.000	1.00	0.00
LEU80	H	1.00	0.000	1.00	0.00
ASP81	H	1.00	0.000	1.00	0.00

## 3.80.9 Detailed Probabilities of LEU80HB3:

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

## 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	0.000	1.00	0.00
LEU80	HB2	1.00	0.000	1.00	0.00
LEU80	HB3	1.00	0.000	1.00	0.00
LEU80	HG	1.00	0.000	1.00	0.00
LEU80	HD11	1.00	0.000	1.00	0.00
LEU80	HD21	1.00	0.000	1.00	0.00
LEU80	H	1.00	0.000	1.00	0.00
ASP81	H	1.00	0.000	1.00	0.00

## 3.80.10 Detailed Probabilities of LEU80HG:

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

**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	0.000	1.00	0.00
LEU80	HB2	1.00	0.000	1.00	0.00
LEU80	HB3	1.00	0.000	1.00	0.00
LEU80	HG	1.00	0.000	1.00	0.00
LEU80	HD11	1.00	0.000	1.00	0.00
LEU80	HD21	1.00	0.000	1.00	0.00
LEU80	H	1.00	0.000	1.00	0.00
ASP81	H	0.97	0.000	1.00	0.00

**3.80.11 Detailed Probabilities of LEU80HD11:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU80	1.00	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	0.000	1.00	0.00
LEU80	HB2	1.00	0.000	1.00	0.00
LEU80	HB3	1.00	0.000	1.00	0.00
LEU80	HG	1.00	0.000	1.00	0.00
LEU80	HD11	1.00	0.000	1.00	0.00
LEU80	HD21	1.00	0.000	1.00	0.00
LEU80	H	0.86	0.000	1.00	0.00

**3.80.12 Detailed Probabilities of LEU80HD21:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU80	1.00	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	0.00
LEU80	HB2	1.00	0.000	1.00	0.00
LEU80	HB3	1.00	0.000	1.00	0.00
LEU80	HG	1.00	0.000	1.00	0.00
LEU80	HD11	1.00	0.000	1.00	0.00
LEU80	HD21	1.00	0.000	1.00	0.00
LEU80	H	0.85	0.000	1.00	0.00

**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	0.000	1.00	0.00
GLU79	HB2	1.00	0.000	1.00	0.00
GLU79	HB3	1.00	0.000	1.00	0.00
GLU79	HG2	0.98	0.000	1.00	0.00
GLU79	HG3	0.97	0.000	1.00	0.00
GLU79	H	1.00	0.000	1.00	0.00
LEU80	HA	1.00	0.000	1.00	0.00
LEU80	HB2	1.00	0.000	1.00	0.00
LEU80	HB3	1.00	0.000	1.00	0.00
LEU80	HG	1.00	0.000	1.00	0.00
LEU80	H	1.00	0.000	1.00	0.00
LEU80	HD11	0.88	0.000	1.00	0.00
LEU80	HD21	0.87	0.000	1.00	0.00
ASP81	H	1.00	0.000	1.00	0.00

**3.81 ASP(81)**

Figure 71: Image from the BMRB

Residue probability: 0.969

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	1.000	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	0.923	1.000
HD2	NA	—	—	0.000	0.000
HA 3.81.4	4.567	4.587	0.329	0.857	0.875
HB2 3.81.5	2.833	2.708	0.282	1.000	0.833
HB3 3.81.6	2.704	2.654	0.285	1.000	0.833
H 3.81.7	8.479	8.304	1.027	1.000	1.000

**3.81.1 Detailed Probabilities of ASP81CA:**

Overall probability: 1.000

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU80	1.00	1.00
ASP81	1.00	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	0.026	1.00	0.00
ASP81	HA	1.00	0.000	1.00	0.00
ASP81	HB2	1.00	0.000	1.00	0.00
ASP81	HB3	1.00	0.000	1.00	0.00
ASP81	H	1.00	0.000	1.00	0.00
TRP82	HA	1.00	0.030	1.00	0.00
TRP82	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ASP81	HB2	1.00	0.000	1.00	0.00
ASP81	HB3	1.00	0.000	1.00	0.00
ASP81	H	1.00	0.000	1.00	0.00
TRP82	H	1.00	0.000	1.00	0.00

**3.81.3 Detailed Probabilities of ASP81N:**

Overall probability: 0.923

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU80	1.00	1.00
ASP81	1.00	1.00
TRP82	0.50	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	0.000	1.00	0.00
LEU80	HB2	1.00	0.000	1.00	0.00
LEU80	HB3	1.00	0.000	1.00	0.00
LEU80	HG	0.97	0.000	1.00	0.00
LEU80	H	1.00	0.000	1.00	0.00
LEU80	HD11	0.54	0.000	1.00	0.00
LEU80	HD21	0.58	0.000	1.00	0.00
ASP81	HA	1.00	0.000	1.00	0.00
ASP81	HB2	1.00	0.000	1.00	0.00
ASP81	HB3	1.00	0.000	1.00	0.00
ASP81	H	1.00	0.000	1.00	0.00
TRP82	H	1.00	0.893	0.00	0.00
TRP82	HA	0.90	0.030	1.00	0.00

**3.81.4 Detailed Probabilities of ASP81HA:**

Overall probability: 0.857

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU80	0.00	1.00
ASP81	1.00	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	0.362	0.00	0.00
ASP81	HA	1.00	0.000	1.00	0.00
ASP81	HB2	1.00	0.000	1.00	0.00
ASP81	HB3	1.00	0.000	1.00	0.00
ASP81	H	1.00	0.000	1.00	0.00
TRP82	HA	1.00	0.030	1.00	0.00
TRP82	H	1.00	0.000	1.00	0.00

**3.81.5 Detailed Probabilities of ASP81HB2:**

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
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	0.000	1.00	0.00
ASP81	HB2	1.00	0.000	1.00	0.00
ASP81	HB3	1.00	0.000	1.00	0.00
ASP81	H	1.00	0.000	1.00	0.00
TRP82	H	1.00	0.000	1.00	0.00

**3.81.6 Detailed Probabilities of ASP81HB3:**

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	0.000	1.00	0.00
ASP81	HB2	1.00	0.000	1.00	0.00
ASP81	HB3	1.00	0.000	1.00	0.00
ASP81	H	1.00	0.000	1.00	0.00
TRP82	H	1.00	0.000	1.00	0.00

**3.81.7 Detailed Probabilities of ASP81H:**

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**

## 3.81 ASP(81)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU80	HA	1.00	0.000	1.00	0.00
LEU80	HB2	1.00	0.000	1.00	0.00
LEU80	HB3	1.00	0.000	1.00	0.00
LEU80	HG	0.97	0.000	1.00	0.00
LEU80	H	1.00	0.000	1.00	0.00
LEU80	HD11	0.54	0.000	1.00	0.00
LEU80	HD21	0.58	0.000	1.00	0.00
ASP81	HA	1.00	0.000	1.00	0.00
ASP81	HB2	1.00	0.000	1.00	0.00
ASP81	HB3	1.00	0.000	1.00	0.00
ASP81	H	1.00	0.000	1.00	0.00
TRP82	H	1.00	0.000	1.00	0.00

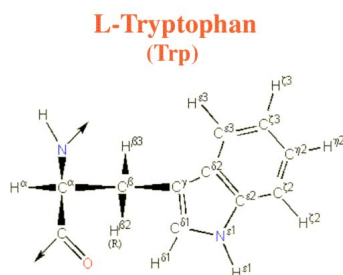
**3.82 TRP(82)**

Figure 72: Image from the BMRB

Residue probability: 0.770

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	0.889	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	0.750	1.000
CE3 3.82.4	120.380	120.123	5.387	0.667	1.000
CZ2 3.82.5	115.636	114.015	4.831	0.667	1.000
CZ3 3.82.6	120.286	121.013	5.400	0.750	1.000
CH2 3.82.7	124.501	123.568	4.896	0.600	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	0.750	1.000
HA 3.82.10	4.597	4.675	0.550	1.000	1.000
HB2 3.82.11	3.343	3.173	0.355	0.875	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	0.625	1.000
HE3 3.82.14	7.658	7.268	0.457	0.556	1.000
HZ2 3.82.15	7.353	7.261	0.347	0.500	1.000
HZ3 3.82.16	6.829	6.836	0.396	1.000	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	0.800	1.000
HE1 3.82.19	9.809	10.060	0.770	0.429	1.000

**3.82.1 Detailed Probabilities of TRP82CA:**

Overall probability: 0.889

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASP81	1.00	1.00
TRP82	0.83	1.00
ASN83	1.00	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	0.030	1.00	0.00
TRP82	HA	1.00	0.000	1.00	0.00
TRP82	HB2	1.00	0.000	1.00	0.00
TRP82	HB3	1.00	0.000	1.00	0.00
TRP82	HD1	1.00	0.117	0.00	0.00
TRP82	HE3	1.00	0.000	1.00	0.00
TRP82	H	1.00	0.000	1.00	0.00
ASN83	HA	1.00	0.030	1.00	0.00
ASN83	H	1.00	0.000	1.00	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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TRP82	HA	1.00	0.000	1.00	0.00
TRP82	HB2	1.00	0.000	1.00	0.00
TRP82	HB3	1.00	0.000	1.00	0.00
TRP82	HD1	1.00	0.001	1.00	0.00
TRP82	HE3	1.00	0.000	1.00	0.00
TRP82	H	1.00	0.000	1.00	0.00
TRP82	HE1	1.00	0.437	0.00	0.00
ASN83	H	1.00	0.289	0.00	0.00
ASN83	HA	0.63	0.030	1.00	0.00

## 3.82.3 Detailed Probabilities of TRP82CD1:

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	0.000	1.00	0.00
TRP82	HB2	1.00	0.000	1.00	0.00
TRP82	HB3	1.00	0.000	1.00	0.00
TRP82	HD1	1.00	0.001	1.00	0.00
TRP82	HE3	1.00	0.123	0.00	0.00
TRP82	HZ2	1.00	0.180	0.00	0.00
TRP82	H	0.99	0.000	1.00	0.00
TRP82	HE1	1.00	0.000	1.00	0.00

## 3.82.4 Detailed Probabilities of TRP82CE3:

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
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	0.000	1.00	0.00
TRP82	HB2	1.00	0.000	1.00	0.00
TRP82	HB3	1.00	0.000	1.00	0.00
TRP82	HD1	1.00	0.106	0.00	0.00
TRP82	HE3	1.00	0.000	1.00	0.00
TRP82	HZ2	1.00	0.075	0.00	0.00
TRP82	HZ3	1.00	0.004	1.00	0.00
TRP82	HH2	1.00	0.001	1.00	0.00
TRP82	HE1	1.00	2.151	0.00	0.00

**3.82.5 Detailed Probabilities of TRP82CZ2:**

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	0.180	0.00	0.00
TRP82	HE3	1.00	0.304	0.00	0.00
TRP82	HZ2	1.00	0.001	1.00	0.00
TRP82	HZ3	1.00	0.004	1.00	0.00
TRP82	HH2	1.00	0.001	1.00	0.00
TRP82	HE1	1.00	0.000	1.00	0.00

**3.82.6 Detailed Probabilities of TRP82CZ3:**

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	0.00
TRP82	HZ2	1.00	0.161	0.00	0.00
TRP82	HZ3	1.00	0.004	1.00	0.00
TRP82	HH2	1.00	0.001	1.00	0.00

**3.82.7 Detailed Probabilities of TRP82CH2:**

Overall probability: 0.600

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
TRP82	0.60	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	0.304	0.00	0.00
TRP82	HZ2	1.00	0.001	1.00	0.00
TRP82	HZ3	1.00	0.004	1.00	0.00
TRP82	HH2	1.00	0.001	1.00	0.00
TRP82	HE1	1.00	0.327	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	0.000	1.00	0.00
ASP81	HB2	1.00	0.000	1.00	0.00
ASP81	HB3	1.00	0.000	1.00	0.00
ASP81	H	1.00	0.000	1.00	0.00
TRP82	HA	1.00	0.000	1.00	0.00
TRP82	HB2	1.00	0.000	1.00	0.00
TRP82	HB3	1.00	0.000	1.00	0.00
TRP82	HD1	0.99	0.001	1.00	0.00
TRP82	H	1.00	0.000	1.00	0.00
ASN83	H	1.00	0.000	1.00	0.00
ASN83	HA	0.85	0.000	1.00	0.00

**3.82.9 Detailed Probabilities of TRP82NE1:**

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
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	0.148	0.00	0.00
TRP82	HB3	1.00	0.000	1.00	0.00
TRP82	HD1	1.00	0.001	1.00	0.00
TRP82	HE3	1.00	0.123	0.00	0.00
TRP82	HZ2	1.00	0.002	1.00	0.00
TRP82	HH2	1.00	0.001	1.00	0.00
TRP82	HE1	1.00	0.000	1.00	0.00
TRP82	HA	0.60	0.000	1.00	0.00

**3.82.10 Detailed Probabilities of TRP82HA:**

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
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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP81	HA	1.00	0.030	1.00	0.00
ASP81	HB2	0.61	0.030	1.00	0.00
ASP81	HB3	0.86	0.030	1.00	0.00
ASP81	H	0.90	0.030	1.00	0.00
TRP82	HA	1.00	0.000	1.00	0.00
TRP82	HB2	1.00	0.000	1.00	0.00
TRP82	HB3	1.00	0.000	1.00	0.00
TRP82	HD1	1.00	0.000	1.00	0.00
TRP82	HE3	1.00	0.000	1.00	0.00
TRP82	H	1.00	0.000	1.00	0.00
TRP82	HE1	0.60	0.000	1.00	0.00
ASN83	HA	1.00	0.030	1.00	0.00
ASN83	H	1.00	0.000	1.00	0.00

## 3.82.11 Detailed Probabilities of TRP82HB2:

Overall probability: 0.875

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	0.000	1.00	0.00
TRP82	HB2	1.00	0.000	1.00	0.00
TRP82	HB3	1.00	0.000	1.00	0.00
TRP82	HD1	1.00	0.000	1.00	0.00
TRP82	HE3	1.00	0.000	1.00	0.00
TRP82	H	1.00	0.000	1.00	0.00
TRP82	HE1	1.00	0.148	0.00	0.00
ASN83	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
TRP82	HB2	1.00	0.000	1.00	0.00
TRP82	HB3	1.00	0.000	1.00	0.00
TRP82	HD1	1.00	0.000	1.00	0.00
TRP82	HE3	1.00	0.000	1.00	0.00
TRP82	H	1.00	0.000	1.00	0.00
TRP82	HE1	1.00	0.000	1.00	0.00
ASN83	H	1.00	0.000	1.00	0.00

**3.82.13 Detailed Probabilities of TRP82HD1:**

Overall probability: 0.625

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
TRP82	0.62	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	0.117	0.00	0.00
TRP82	HB2	1.00	0.001	1.00	0.00
TRP82	HB3	1.00	0.001	1.00	0.00
TRP82	HD1	1.00	0.001	1.00	0.00
TRP82	HE3	1.00	0.106	0.00	0.00
TRP82	HZ2	1.00	0.180	0.00	0.00
TRP82	H	0.99	0.001	1.00	0.00
TRP82	HE1	1.00	0.001	1.00	0.00

**3.82.14 Detailed Probabilities of TRP82HE3:**

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	0.000	1.00	0.00
TRP82	HB2	1.00	0.000	1.00	0.00
TRP82	HB3	1.00	0.000	1.00	0.00
TRP82	HD1	1.00	0.123	0.00	0.00
TRP82	HE3	1.00	0.000	1.00	0.00
TRP82	HZ2	1.00	0.304	0.00	0.00
TRP82	HZ3	1.00	0.000	1.00	0.00
TRP82	HH2	1.00	0.304	0.00	0.00
TRP82	HE1	1.00	0.123	0.00	0.00

**3.82.15 Detailed Probabilities of TRP82HZ2:**

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
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	0.180	0.00	0.00
TRP82	HE3	1.00	0.075	0.00	0.00
TRP82	HZ2	1.00	0.001	1.00	0.00
TRP82	HZ3	1.00	0.161	0.00	0.00
TRP82	HH2	1.00	0.001	1.00	0.00
TRP82	HE1	1.00	0.002	1.00	0.00

**3.82.16 Detailed Probabilities of TRP82HZ3:**

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
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	0.004	1.00	0.00
TRP82	HZ2	1.00	0.004	1.00	0.00
TRP82	HZ3	1.00	0.004	1.00	0.00
TRP82	HH2	1.00	0.004	1.00	0.00

**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	0.00
TRP82	HZ2	1.00	0.001	1.00	0.00
TRP82	HZ3	1.00	0.001	1.00	0.00
TRP82	HH2	1.00	0.001	1.00	0.00
TRP82	HE1	1.00	0.001	1.00	0.00

**3.82.18 Detailed Probabilities of TRP82H:**

Overall probability: 0.800

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASP81	0.50	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	0.000	1.00	0.00
ASP81	HB2	1.00	0.893	0.00	0.00
ASP81	HB3	1.00	0.000	1.00	0.00
ASP81	H	1.00	0.893	0.00	0.00
TRP82	HA	1.00	0.000	1.00	0.00
TRP82	HB2	1.00	0.000	1.00	0.00
TRP82	HB3	1.00	0.000	1.00	0.00
TRP82	HD1	0.99	0.000	1.00	0.00
TRP82	H	1.00	0.000	1.00	0.00
ASN83	H	1.00	0.000	1.00	0.00

**3.82.19 Detailed Probabilities of TRP82HE1:**

Overall probability: 0.429

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
TRP82	0.43	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	0.437	0.00	0.00
TRP82	HB3	1.00	0.437	0.00	0.00
TRP82	HD1	1.00	0.000	1.00	0.00
TRP82	HE3	1.00	2.151	0.00	0.00
TRP82	HZ2	1.00	0.000	1.00	0.00
TRP82	HH2	1.00	0.327	0.00	0.00
TRP82	HE1	1.00	0.000	1.00	0.00

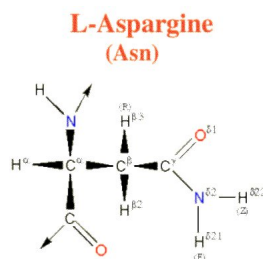
**3.83 ASN(83)**

Figure 73: Image from the BMRB

Residue probability: 0.964

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	0.900	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	1.000	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	0.923	1.000
HB2 3.83.6	2.956	2.800	0.341	1.000	1.000
HB3 3.83.7	2.772	2.739	0.364	1.000	1.000
H 3.83.8	9.661	8.328	0.633	0.818	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	1.000	1.000

**3.83.1 Detailed Probabilities of ASN83CA:**

Overall probability: 0.900

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
TRP82	1.00	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	0.030	1.00	0.00
ASN83	HA	1.00	0.000	1.00	0.00
ASN83	HB2	1.00	0.000	1.00	0.00
ASN83	HB3	1.00	0.000	1.00	0.00
ASN83	H	1.00	0.000	1.00	0.00
ASN83	HD21	1.00	0.000	1.00	0.00
ASN83	HD22	1.00	0.000	1.00	0.00
LEU84	HA	1.00	0.162	0.00	0.00
LEU84	H	1.00	0.000	1.00	0.00
LEU84	HB2	0.52	0.029	1.00	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	0.000	1.00	0.00
ASN83	HB2	1.00	0.000	1.00	0.00
ASN83	HB3	1.00	0.000	1.00	0.00
ASN83	H	1.00	0.000	1.00	0.00
ASN83	HD21	1.00	0.000	1.00	0.00
ASN83	HD22	1.00	0.000	1.00	0.00
LEU84	H	1.00	0.000	1.00	0.00

**3.83.3 Detailed Probabilities of ASN83N:**

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
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	0.000	1.00	0.00
TRP82	HB2	1.00	0.000	1.00	0.00
TRP82	HB3	1.00	0.000	1.00	0.00
TRP82	H	1.00	0.000	1.00	0.00
ASN83	HA	1.00	0.000	1.00	0.00
ASN83	HB2	1.00	0.000	1.00	0.00
ASN83	HB3	1.00	0.000	1.00	0.00
ASN83	H	1.00	0.000	1.00	0.00
ASN83	HD21	0.98	0.004	1.00	0.00
LEU84	H	1.00	0.000	1.00	0.00
LEU84	HB2	0.65	0.012	1.00	0.00

**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	0.000	1.00	0.00
ASN83	HB2	1.00	0.000	1.00	0.00
ASN83	HB3	1.00	0.000	1.00	0.00
ASN83	H	0.98	0.011	1.00	0.00
ASN83	HD21	1.00	0.000	1.00	0.00
ASN83	HD22	1.00	0.000	1.00	0.00

**3.83.5 Detailed Probabilities of ASN83HA:**

Overall probability: 0.923

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
TRP82	1.00	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	0.030	1.00	0.00
TRP82	HB2	0.63	0.030	1.00	0.00
TRP82	HB3	0.81	0.030	1.00	0.00
TRP82	H	0.85	0.000	1.00	0.00
ASN83	HA	1.00	0.000	1.00	0.00
ASN83	HB2	1.00	0.000	1.00	0.00
ASN83	HB3	1.00	0.000	1.00	0.00
ASN83	H	1.00	0.000	1.00	0.00
ASN83	HD21	1.00	0.000	1.00	0.00
ASN83	HD22	1.00	0.000	1.00	0.00
LEU84	HA	1.00	0.148	0.00	0.00
LEU84	H	1.00	0.000	1.00	0.00
LEU84	HB2	0.52	0.018	1.00	0.00

**3.83.6 Detailed Probabilities of ASN83HB2:**

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	0.000	1.00	0.00
ASN83	HB2	1.00	0.000	1.00	0.00
ASN83	HB3	1.00	0.000	1.00	0.00
ASN83	H	1.00	0.000	1.00	0.00
ASN83	HD21	1.00	0.000	1.00	0.00
ASN83	HD22	1.00	0.000	1.00	0.00
LEU84	H	1.00	0.000	1.00	0.00

**3.83.7 Detailed Probabilities of ASN83HB3:**

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
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	0.00
ASN83	HB2	1.00	0.000	1.00	0.00
ASN83	HB3	1.00	0.000	1.00	0.00
ASN83	H	1.00	0.000	1.00	0.00
ASN83	HD21	1.00	0.000	1.00	0.00
ASN83	HD22	1.00	0.000	1.00	0.00
LEU84	H	1.00	0.000	1.00	0.00

**3.83.8 Detailed Probabilities of ASN83H:**

Overall probability: 0.818

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
TRP82	0.50	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	0.000	1.00	0.00
TRP82	HB2	1.00	0.289	0.00	0.00
TRP82	HB3	1.00	0.289	0.00	0.00
TRP82	H	1.00	0.000	1.00	0.00
ASN83	HA	1.00	0.000	1.00	0.00
ASN83	HB2	1.00	0.000	1.00	0.00
ASN83	HB3	1.00	0.000	1.00	0.00
ASN83	H	1.00	0.000	1.00	0.00
ASN83	HD21	0.98	0.011	1.00	0.00
ASN83	HD22	0.63	0.020	1.00	0.00
LEU84	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ASN83	HB2	1.00	0.000	1.00	0.00
ASN83	HB3	1.00	0.000	1.00	0.00
ASN83	H	0.98	0.004	1.00	0.00
ASN83	HD21	1.00	0.000	1.00	0.00
ASN83	HD22	1.00	0.000	1.00	0.00

**3.83.10 Detailed Probabilities of ASN83HD22:**

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
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	0.000	1.00	0.00
ASN83	HB2	1.00	0.000	1.00	0.00
ASN83	HB3	1.00	0.000	1.00	0.00
ASN83	HD21	1.00	0.000	1.00	0.00
ASN83	HD22	1.00	0.000	1.00	0.00

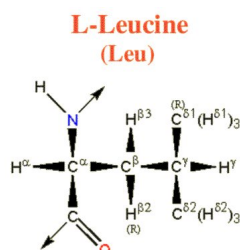
**3.84 LEU(84)**

Figure 74: Image from the BMRB

Residue probability: 0.971

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	0.800	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	1.000	1.000
N 3.84.6	117.468	121.785	4.943	1.000	1.000
HA 3.84.7	4.405	4.315	0.840	0.818	1.000
HB2 3.84.8	1.727	1.601	0.373	1.000	1.000
HB3 3.84.9	1.947	1.508	0.398	1.000	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	1.000	1.000
H 3.84.13	7.784	8.237	0.647	1.000	1.000

**3.84.1 Detailed Probabilities of LEU84CA:**

Overall probability: 0.800

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASN83	0.00	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	0.148	0.00	0.00
LEU84	HA	1.00	0.000	1.00	0.00
LEU84	HB2	1.00	0.000	1.00	0.00
LEU84	HB3	1.00	0.000	1.00	0.00
LEU84	HG	1.00	0.000	1.00	0.00
LEU84	HD11	0.99	0.000	1.00	0.00
LEU84	HD21	0.99	0.000	1.00	0.00
LEU84	H	1.00	0.000	1.00	0.00
LEU85	HA	1.00	0.185	0.00	0.00
LEU85	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
LEU84	HB2	1.00	0.000	1.00	0.00
LEU84	HB3	1.00	0.000	1.00	0.00
LEU84	HG	1.00	0.000	1.00	0.00
LEU84	HD11	1.00	0.000	1.00	0.00
LEU84	HD21	1.00	0.000	1.00	0.00
LEU84	H	1.00	0.000	1.00	0.00
LEU85	H	1.00	0.000	1.00	0.00
LEU85	HA	0.65	0.019	1.00	0.00

## 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	0.000	1.00	0.00
LEU84	HB2	1.00	0.000	1.00	0.00
LEU84	HB3	1.00	0.000	1.00	0.00
LEU84	HG	1.00	0.000	1.00	0.00
LEU84	HD11	1.00	0.000	1.00	0.00
LEU84	HD21	1.00	0.000	1.00	0.00
LEU84	H	1.00	0.000	1.00	0.00
LEU85	H	0.98	0.000	1.00	0.00

## 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	0.000	1.00	0.00
LEU84	HB2	1.00	0.000	1.00	0.00
LEU84	HB3	1.00	0.000	1.00	0.00
LEU84	HG	1.00	0.000	1.00	0.00
LEU84	HD11	1.00	0.000	1.00	0.00
LEU84	HD21	1.00	0.000	1.00	0.00
LEU84	H	0.86	0.000	1.00	0.00

**3.84.5 Detailed Probabilities of LEU84CD2:**

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
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	0.000	1.00	0.00
LEU84	HB2	1.00	0.000	1.00	0.00
LEU84	HB3	1.00	0.000	1.00	0.00
LEU84	HG	1.00	0.000	1.00	0.00
LEU84	HD11	1.00	0.000	1.00	0.00
LEU84	HD21	1.00	0.000	1.00	0.00
LEU84	H	0.85	0.000	1.00	0.00

**3.84.6 Detailed Probabilities of LEU84N:**

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
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	0.000	1.00	0.00
ASN83	HB2	1.00	0.000	1.00	0.00
ASN83	HB3	1.00	0.000	1.00	0.00
ASN83	H	1.00	0.000	1.00	0.00
LEU84	HA	1.00	0.000	1.00	0.00
LEU84	HB2	1.00	0.000	1.00	0.00
LEU84	HB3	1.00	0.000	1.00	0.00
LEU84	HG	1.00	0.000	1.00	0.00
LEU84	H	1.00	0.000	1.00	0.00
LEU84	HD11	0.88	0.000	1.00	0.00
LEU84	HD21	0.87	0.000	1.00	0.00
LEU85	H	1.00	0.000	1.00	0.00

**3.84.7 Detailed Probabilities of LEU84HA:**

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	0.162	0.00	0.00
ASN83	HB3	0.87	0.005	1.00	0.00
LEU84	HA	1.00	0.000	1.00	0.00
LEU84	HB2	1.00	0.000	1.00	0.00
LEU84	HB3	1.00	0.000	1.00	0.00
LEU84	HG	1.00	0.000	1.00	0.00
LEU84	HD11	0.99	0.000	1.00	0.00
LEU84	HD21	0.99	0.000	1.00	0.00
LEU84	H	1.00	0.000	1.00	0.00
LEU85	HA	1.00	0.199	0.00	0.00
LEU85	H	1.00	0.000	1.00	0.00

**3.84.8 Detailed Probabilities of LEU84HB2:**

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	0.000	1.00	0.00
LEU84	HB2	1.00	0.000	1.00	0.00
LEU84	HB3	1.00	0.000	1.00	0.00
LEU84	HG	1.00	0.000	1.00	0.00
LEU84	HD11	1.00	0.000	1.00	0.00
LEU84	HD21	1.00	0.000	1.00	0.00
LEU84	H	1.00	0.000	1.00	0.00
LEU85	H	1.00	0.000	1.00	0.00

## 3.84.9 Detailed Probabilities of LEU84HB3:

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
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	0.000	1.00	0.00
LEU84	HB2	1.00	0.000	1.00	0.00
LEU84	HB3	1.00	0.000	1.00	0.00
LEU84	HG	1.00	0.000	1.00	0.00
LEU84	HD11	1.00	0.000	1.00	0.00
LEU84	HD21	1.00	0.000	1.00	0.00
LEU84	H	1.00	0.000	1.00	0.00
LEU85	H	1.00	0.000	1.00	0.00

## 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	0.000	1.00	0.00
LEU84	HB2	1.00	0.000	1.00	0.00
LEU84	HB3	1.00	0.000	1.00	0.00
LEU84	HG	1.00	0.000	1.00	0.00
LEU84	HD11	1.00	0.000	1.00	0.00
LEU84	HD21	1.00	0.000	1.00	0.00
LEU84	H	1.00	0.000	1.00	0.00
LEU85	H	0.98	0.000	1.00	0.00

**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	0.000	1.00	0.00
LEU84	HB2	1.00	0.000	1.00	0.00
LEU84	HB3	1.00	0.000	1.00	0.00
LEU84	HG	1.00	0.000	1.00	0.00
LEU84	HD11	1.00	0.000	1.00	0.00
LEU84	HD21	1.00	0.000	1.00	0.00
LEU84	H	0.86	0.000	1.00	0.00

**3.84.12 Detailed Probabilities of LEU84HD21:**

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
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	0.000	1.00	0.00
LEU84	HB2	1.00	0.000	1.00	0.00
LEU84	HB3	1.00	0.000	1.00	0.00
LEU84	HG	1.00	0.000	1.00	0.00
LEU84	HD11	1.00	0.000	1.00	0.00
LEU84	HD21	1.00	0.000	1.00	0.00
LEU84	H	0.85	0.000	1.00	0.00

**3.84.13 Detailed Probabilities of LEU84H:**

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
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	0.000	1.00	0.00
ASN83	HB2	1.00	0.000	1.00	0.00
ASN83	HB3	1.00	0.000	1.00	0.00
ASN83	H	1.00	0.000	1.00	0.00
LEU84	HA	1.00	0.000	1.00	0.00
LEU84	HB2	1.00	0.000	1.00	0.00
LEU84	HB3	1.00	0.000	1.00	0.00
LEU84	HG	1.00	0.000	1.00	0.00
LEU84	H	1.00	0.000	1.00	0.00
LEU84	HD11	0.88	0.000	1.00	0.00
LEU84	HD21	0.87	0.000	1.00	0.00
LEU85	H	1.00	0.000	1.00	0.00

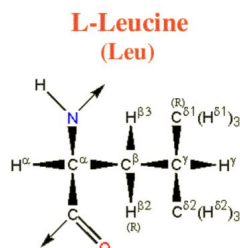


Figure 75: Image from the BMRB

**Residue probability:** 0.971  
**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	0.800	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	1.000	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	1.000	1.000
HA 3.85.7	4.604	4.315	0.840	0.818	1.000
HB2 3.85.8	1.666	1.601	0.373	1.000	1.000
HB3 3.85.9	1.894	1.508	0.398	1.000	1.000
HG 3.85.10	1.678	1.510	0.340	1.000	1.000
HD1 3.85.11	0.611	0.739	0.294	1.000	1.000
HD2 3.85.12	0.789	0.727	0.421	1.000	1.000
H 3.85.13	7.417	8.237	0.647	1.000	1.000

**3.85.1 Detailed Probabilities of LEU85CA:**

**Overall probability:** 0.800  
**Overall confidence:** 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU84	0.00	1.00
LEU85	1.00	1.00
LYS86	0.50	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	0.199	0.00	0.00
LEU85	HA	1.00	0.000	1.00	0.00
LEU85	HB2	1.00	0.000	1.00	0.00
LEU85	HB3	1.00	0.000	1.00	0.00
LEU85	HG	1.00	0.000	1.00	0.00
LEU85	HD11	0.99	0.000	1.00	0.00
LEU85	HD21	0.99	0.000	1.00	0.00
LEU85	H	1.00	0.000	1.00	0.00
LYS86	HA	1.00	0.800	0.00	0.00
LYS86	H	1.00	0.000	1.00	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	0.000	1.00	0.00
LEU85	HB2	1.00	0.000	1.00	0.00
LEU85	HB3	1.00	0.000	1.00	0.00
LEU85	HG	1.00	0.000	1.00	0.00
LEU85	HD11	1.00	0.000	1.00	0.00
LEU85	HD21	1.00	0.000	1.00	0.00
LEU85	H	1.00	0.000	1.00	0.00
LYS86	H	1.00	0.000	1.00	0.00

## 3.85.3 Detailed Probabilities of LEU85CG:

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
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	0.00
LEU85	HB2	1.00	0.000	1.00	0.00
LEU85	HB3	1.00	0.000	1.00	0.00
LEU85	HG	1.00	0.000	1.00	0.00
LEU85	HD11	1.00	0.000	1.00	0.00
LEU85	HD21	1.00	0.000	1.00	0.00
LEU85	H	1.00	0.000	1.00	0.00
LYS86	H	0.98	0.000	1.00	0.00

## 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	0.000	1.00	0.00
LEU85	HB2	1.00	0.000	1.00	0.00
LEU85	HB3	1.00	0.000	1.00	0.00
LEU85	HG	1.00	0.000	1.00	0.00
LEU85	HD11	1.00	0.000	1.00	0.00
LEU85	HD21	1.00	0.000	1.00	0.00
LEU85	H	0.86	0.000	1.00	0.00

**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	0.000	1.00	0.00
LEU85	HB2	1.00	0.000	1.00	0.00
LEU85	HB3	1.00	0.000	1.00	0.00
LEU85	HG	1.00	0.000	1.00	0.00
LEU85	HD11	1.00	0.000	1.00	0.00
LEU85	HD21	1.00	0.000	1.00	0.00
LEU85	H	0.85	0.000	1.00	0.00

**3.85.6 Detailed Probabilities of LEU85N:**

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
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	0.000	1.00	0.00
LEU84	HB2	1.00	0.000	1.00	0.00
LEU84	HB3	1.00	0.000	1.00	0.00
LEU84	HG	0.98	0.000	1.00	0.00
LEU84	H	1.00	0.000	1.00	0.00
LEU84	HD11	0.53	0.000	1.00	0.00
LEU84	HD21	0.58	0.000	1.00	0.00
LEU85	HA	1.00	0.000	1.00	0.00
LEU85	HB2	1.00	0.000	1.00	0.00
LEU85	HB3	1.00	0.000	1.00	0.00
LEU85	HG	1.00	0.000	1.00	0.00
LEU85	H	1.00	0.000	1.00	0.00
LEU85	HD11	0.88	0.000	1.00	0.00
LEU85	HD21	0.87	0.000	1.00	0.00
LYS86	H	1.00	0.000	1.00	0.00
LYS86	HA	0.89	0.018	1.00	0.00
LYS86	HB2	0.58	0.029	1.00	0.00

**3.85.7 Detailed Probabilities of LEU85HA:**

Overall probability: 0.818

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU84	0.50	1.00
LEU85	1.00	1.00
LYS86	0.50	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	0.185	0.00	0.00
LEU84	HB2	0.65	0.019	1.00	0.00
LEU85	HA	1.00	0.000	1.00	0.00
LEU85	HB2	1.00	0.000	1.00	0.00
LEU85	HB3	1.00	0.000	1.00	0.00
LEU85	HG	1.00	0.000	1.00	0.00
LEU85	HD11	0.99	0.000	1.00	0.00
LEU85	HD21	0.99	0.000	1.00	0.00
LEU85	H	1.00	0.000	1.00	0.00
LYS86	HA	1.00	0.800	0.00	0.00
LYS86	H	1.00	0.000	1.00	0.00

**3.85.8 Detailed Probabilities of LEU85HB2:**

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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU85	HA	1.00	0.000	1.00	0.00
LEU85	HB2	1.00	0.000	1.00	0.00
LEU85	HB3	1.00	0.000	1.00	0.00
LEU85	HG	1.00	0.000	1.00	0.00
LEU85	HD11	1.00	0.000	1.00	0.00
LEU85	HD21	1.00	0.000	1.00	0.00
LEU85	H	1.00	0.000	1.00	0.00
LYS86	H	1.00	0.000	1.00	0.00

**3.85.9 Detailed Probabilities of LEU85HB3:**

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
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	0.000	1.00	0.00
LEU85	HB2	1.00	0.000	1.00	0.00
LEU85	HB3	1.00	0.000	1.00	0.00
LEU85	HG	1.00	0.000	1.00	0.00
LEU85	HD11	1.00	0.000	1.00	0.00
LEU85	HD21	1.00	0.000	1.00	0.00
LEU85	H	1.00	0.000	1.00	0.00
LYS86	H	1.00	0.000	1.00	0.00

**3.85.10 Detailed Probabilities of LEU85HG:**

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
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	0.00
LEU85	HB2	1.00	0.000	1.00	0.00
LEU85	HB3	1.00	0.000	1.00	0.00
LEU85	HG	1.00	0.000	1.00	0.00
LEU85	HD11	1.00	0.000	1.00	0.00
LEU85	HD21	1.00	0.000	1.00	0.00
LEU85	H	1.00	0.000	1.00	0.00
LYS86	H	0.98	0.000	1.00	0.00

**3.85.11 Detailed Probabilities of LEU85HD11:**

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	0.000	1.00	0.00
LEU85	HB2	1.00	0.000	1.00	0.00
LEU85	HB3	1.00	0.000	1.00	0.00
LEU85	HG	1.00	0.000	1.00	0.00
LEU85	HD11	1.00	0.000	1.00	0.00
LEU85	HD21	1.00	0.000	1.00	0.00
LEU85	H	0.86	0.000	1.00	0.00

**3.85.12 Detailed Probabilities of LEU85HD21:**

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	0.000	1.00	0.00
LEU85	HB2	1.00	0.000	1.00	0.00
LEU85	HB3	1.00	0.000	1.00	0.00
LEU85	HG	1.00	0.000	1.00	0.00
LEU85	HD11	1.00	0.000	1.00	0.00
LEU85	HD21	1.00	0.000	1.00	0.00
LEU85	H	0.85	0.000	1.00	0.00

**3.85.13 Detailed Probabilities of LEU85H:**

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
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	0.000	1.00	0.00
LEU84	HB2	1.00	0.000	1.00	0.00
LEU84	HB3	1.00	0.000	1.00	0.00
LEU84	HG	0.98	0.000	1.00	0.00
LEU84	H	1.00	0.000	1.00	0.00
LEU84	HD11	0.53	0.000	1.00	0.00
LEU84	HD21	0.58	0.000	1.00	0.00
LEU85	HA	1.00	0.000	1.00	0.00
LEU85	HB2	1.00	0.000	1.00	0.00
LEU85	HB3	1.00	0.000	1.00	0.00
LEU85	HG	1.00	0.000	1.00	0.00
LEU85	H	1.00	0.000	1.00	0.00
LEU85	HD11	0.88	0.000	1.00	0.00
LEU85	HD21	0.87	0.000	1.00	0.00
LYS86	H	1.00	0.000	1.00	0.00

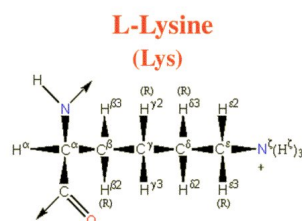


Figure 76: Image from the BMRB

**Residue probability:** 0.958  
**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	0.692	1.000
CB 3.86.2	30.740	32.981	3.186	0.969	1.000
CG 3.86.3	27.210	24.941	1.956	1.000	0.909
CD 3.86.4	29.454	29.020	2.193	1.000	0.900
CE 3.86.5	41.525	41.893	1.492	1.000	0.889
N 3.86.6	116.742	120.954	4.210	1.000	1.000
NZ	NA	—	—	0.000	0.000
HA 3.86.7	3.804	4.262	0.489	0.769	1.000
HB2 3.86.8	1.756	1.774	0.365	1.000	1.000
HB3 3.86.9	1.962	1.742	0.385	1.000	1.000
HG2 3.86.10	1.252	1.358	0.344	1.000	0.909
HG3 3.86.11	1.962	1.343	0.357	1.000	0.909
HD2 3.86.12	1.706	1.614	0.957	1.000	0.900
HD3 3.86.13	1.704	1.595	0.387	1.000	0.900
HE2 3.86.14	2.802	2.907	0.230	0.900	0.889
HE3 3.86.15	2.768	2.901	0.241	1.000	0.889
H 3.86.16	8.659	8.185	0.605	1.000	1.000
HZ	NA	—	—	0.000	0.000

**3.86.1 Detailed Probabilities of LYS86CA:**

**Overall probability:** 0.692  
**Overall confidence:** 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU85	0.00	1.00
LYS86	1.00	1.00
PRO87	0.25	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	0.800	0.00	0.00
LYS86	HA	1.00	0.000	1.00	0.00
LYS86	HB2	1.00	0.000	1.00	0.00
LYS86	HB3	1.00	0.000	1.00	0.00
LYS86	HG2	1.00	0.000	1.00	0.00
LYS86	HG3	1.00	0.000	1.00	0.00
LYS86	HD2	0.98	0.000	1.00	0.00
LYS86	HD3	0.98	0.000	1.00	0.00
LYS86	H	1.00	0.000	1.00	0.00
PRO87	HA	1.00	0.483	0.00	0.00
PRO87	HD2	1.00	0.147	0.00	0.00
PRO87	HD3	1.00	0.248	0.00	0.00
PRO87	HG2	0.93	0.008	1.00	0.00

**3.86.2 Detailed Probabilities of LYS86CB:**

Overall probability: 0.969

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS86	0.96	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	0.000	1.00	0.00
LYS86	HB2	1.00	0.000	1.00	0.00
LYS86	HB3	1.00	0.000	1.00	0.00
LYS86	HG2	1.00	0.000	1.00	0.00
LYS86	HG3	1.00	0.000	1.00	0.00
LYS86	HD2	1.00	0.000	1.00	0.00
LYS86	HD3	1.00	0.000	1.00	0.00
LYS86	HE2	0.99	0.034	0.60	0.00
LYS86	HE3	0.99	0.000	1.00	0.00
LYS86	H	1.00	0.000	1.00	0.00
PRO87	HD2	0.99	0.007	1.00	0.00
PRO87	HD3	1.00	0.003	1.00	0.00
PRO87	HG2	0.53	0.008	1.00	0.00

**3.86.3 Detailed Probabilities of LYS86CG:**

Overall probability: 1.000

Overall confidence: 0.909

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS86	1.00	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	0.000	1.00	0.00
LYS86	HB2	1.00	0.000	1.00	0.00
LYS86	HB3	1.00	0.000	1.00	0.00
LYS86	HG2	1.00	0.000	1.00	0.00
LYS86	HG3	1.00	0.000	1.00	0.00
LYS86	HD2	1.00	0.000	1.00	0.00
LYS86	HD3	1.00	0.000	1.00	0.00
LYS86	HE2	1.00	0.000	1.00	0.00
LYS86	HE3	1.00	0.000	1.00	0.00
LYS86	H	1.00	0.000	1.00	0.00

**3.86.4 Detailed Probabilities of LYS86CD:**

Overall probability: 1.000

Overall confidence: 0.900

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS86	1.00	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	0.000	1.00	0.00
LYS86	HB2	1.00	0.000	1.00	0.00
LYS86	HB3	1.00	0.000	1.00	0.00
LYS86	HG2	1.00	0.000	1.00	0.00
LYS86	HG3	1.00	0.000	1.00	0.00
LYS86	HD2	1.00	0.000	1.00	0.00
LYS86	HD3	1.00	0.000	1.00	0.00
LYS86	HE2	1.00	0.000	1.00	0.00
LYS86	HE3	1.00	0.000	1.00	0.00
LYS86	H	0.88	0.000	1.00	0.00

**3.86.5 Detailed Probabilities of LYS86CE:**

Overall probability: 1.000

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS86	1.00	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	0.000	1.00	0.00
LYS86	HB3	0.99	0.000	1.00	0.00
LYS86	HG2	1.00	0.000	1.00	0.00
LYS86	HG3	1.00	0.000	1.00	0.00
LYS86	HD2	1.00	0.000	1.00	0.00
LYS86	HD3	1.00	0.000	1.00	0.00
LYS86	HE2	1.00	0.000	1.00	0.00
LYS86	HE3	1.00	0.000	1.00	0.00

**3.86.6 Detailed Probabilities of LYS86N:**

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
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	0.000	1.00	0.00
LEU85	HB2	1.00	0.000	1.00	0.00
LEU85	HB3	1.00	0.000	1.00	0.00
LEU85	HG	0.98	0.000	1.00	0.00
LEU85	H	1.00	0.000	1.00	0.00
LEU85	HD11	0.52	0.000	1.00	0.00
LEU85	HD21	0.59	0.000	1.00	0.00
LYS86	HA	1.00	0.000	1.00	0.00
LYS86	HB2	1.00	0.000	1.00	0.00
LYS86	HB3	1.00	0.000	1.00	0.00
LYS86	HG2	1.00	0.000	1.00	0.00
LYS86	HG3	1.00	0.000	1.00	0.00
LYS86	H	1.00	0.000	1.00	0.00
LYS86	HD2	0.88	0.000	1.00	0.00
LYS86	HD3	0.87	0.000	1.00	0.00
PRO87	HD2	0.99	0.015	1.00	0.00
PRO87	HD3	0.99	0.003	1.00	0.00

**3.86.7 Detailed Probabilities of LYS86HA:**

Overall probability: 0.769

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU85	0.50	1.00
LYS86	1.00	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	0.800	0.00	0.00
LEU85	H	0.89	0.018	1.00	0.00
LYS86	HA	1.00	0.000	1.00	0.00
LYS86	HB2	1.00	0.000	1.00	0.00
LYS86	HB3	1.00	0.000	1.00	0.00
LYS86	HG2	1.00	0.000	1.00	0.00
LYS86	HG3	1.00	0.000	1.00	0.00
LYS86	HD2	0.98	0.000	1.00	0.00
LYS86	HD3	0.98	0.000	1.00	0.00
LYS86	H	1.00	0.000	1.00	0.00
PRO87	HA	1.00	0.147	0.00	0.00
PRO87	HD2	1.00	0.137	0.00	0.00
PRO87	HD3	1.00	0.000	1.00	0.00

**3.86.8 Detailed Probabilities of LYS86HB2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS86	1.00	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	0.000	1.00	0.00
LYS86	HB2	1.00	0.000	1.00	0.00
LYS86	HB3	1.00	0.000	1.00	0.00
LYS86	HG2	1.00	0.000	1.00	0.00
LYS86	HG3	1.00	0.000	1.00	0.00
LYS86	HD2	1.00	0.000	1.00	0.00
LYS86	HD3	1.00	0.000	1.00	0.00
LYS86	HE2	0.98	0.000	1.00	0.00
LYS86	HE3	0.99	0.000	1.00	0.00
LYS86	H	1.00	0.000	1.00	0.00
PRO87	HD2	0.99	0.016	1.00	0.00
PRO87	HD3	1.00	0.020	1.00	0.00

**3.86.9 Detailed Probabilities of LYS86HB3:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS86	1.00	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	0.000	1.00	0.00
LYS86	HB2	1.00	0.000	1.00	0.00
LYS86	HB3	1.00	0.000	1.00	0.00
LYS86	HG2	1.00	0.000	1.00	0.00
LYS86	HG3	1.00	0.000	1.00	0.00
LYS86	HD2	1.00	0.000	1.00	0.00
LYS86	HD3	1.00	0.000	1.00	0.00
LYS86	HE2	0.99	0.000	1.00	0.00
LYS86	HE3	0.99	0.000	1.00	0.00
LYS86	H	1.00	0.000	1.00	0.00
PRO87	HD2	0.99	0.008	1.00	0.00
PRO87	HD3	1.00	0.008	1.00	0.00
PRO87	HA	0.80	0.008	1.00	0.00
PRO87	HG2	0.53	0.008	1.00	0.00

**3.86.10 Detailed Probabilities of LYS86HG2:**

Overall probability: 1.000

Overall confidence: 0.909

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS86	1.00	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	0.000	1.00	0.00
LYS86	HB2	1.00	0.000	1.00	0.00
LYS86	HB3	1.00	0.000	1.00	0.00
LYS86	HG2	1.00	0.000	1.00	0.00
LYS86	HG3	1.00	0.000	1.00	0.00
LYS86	HD2	1.00	0.000	1.00	0.00
LYS86	HD3	1.00	0.000	1.00	0.00
LYS86	HE2	1.00	0.000	1.00	0.00
LYS86	HE3	1.00	0.000	1.00	0.00
LYS86	H	1.00	0.000	1.00	0.00

**3.86.11 Detailed Probabilities of LYS86HG3:**

Overall probability: 1.000

Overall confidence: 0.909

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS86	1.00	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	0.000	1.00	0.00
LYS86	HB2	1.00	0.000	1.00	0.00
LYS86	HB3	1.00	0.000	1.00	0.00
LYS86	HG2	1.00	0.000	1.00	0.00
LYS86	HG3	1.00	0.000	1.00	0.00
LYS86	HD2	1.00	0.000	1.00	0.00
LYS86	HD3	1.00	0.000	1.00	0.00
LYS86	HE2	1.00	0.000	1.00	0.00
LYS86	HE3	1.00	0.000	1.00	0.00
LYS86	H	1.00	0.000	1.00	0.00

**3.86.12 Detailed Probabilities of LYS86HD2:**

Overall probability: 1.000

Overall confidence: 0.900

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS86	1.00	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	0.000	1.00	0.00
LYS86	HB2	1.00	0.000	1.00	0.00
LYS86	HB3	1.00	0.000	1.00	0.00
LYS86	HG2	1.00	0.000	1.00	0.00
LYS86	HG3	1.00	0.000	1.00	0.00
LYS86	HD2	1.00	0.000	1.00	0.00
LYS86	HD3	1.00	0.000	1.00	0.00
LYS86	HE2	1.00	0.000	1.00	0.00
LYS86	HE3	1.00	0.000	1.00	0.00
LYS86	H	0.88	0.000	1.00	0.00

**3.86.13 Detailed Probabilities of LYS86HD3:**

Overall probability: 1.000

Overall confidence: 0.900

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS86	1.00	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	0.000	1.00	0.00
LYS86	HB2	1.00	0.000	1.00	0.00
LYS86	HB3	1.00	0.000	1.00	0.00
LYS86	HG2	1.00	0.000	1.00	0.00
LYS86	HG3	1.00	0.000	1.00	0.00
LYS86	HD2	1.00	0.000	1.00	0.00
LYS86	HD3	1.00	0.000	1.00	0.00
LYS86	HE2	1.00	0.000	1.00	0.00
LYS86	HE3	1.00	0.000	1.00	0.00
LYS86	H	0.87	0.000	1.00	0.00

## 3.86.14 Detailed Probabilities of LYS86HE2:

Overall probability: 0.900

Overall confidence: 0.889

## Inter- and intra-residue probability

Residue	Probability	Confidence
LYS86	0.90	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	0.034	0.60	0.00
LYS86	HB3	0.99	0.034	0.60	0.00
LYS86	HG2	1.00	0.000	1.00	0.00
LYS86	HG3	1.00	0.000	1.00	0.00
LYS86	HD2	1.00	0.000	1.00	0.00
LYS86	HD3	1.00	0.000	1.00	0.00
LYS86	HE2	1.00	0.000	1.00	0.00
LYS86	HE3	1.00	0.000	1.00	0.00

## 3.86.15 Detailed Probabilities of LYS86HE3:

Overall probability: 1.000

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS86	1.00	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	0.000	1.00	0.00
LYS86	HB3	0.99	0.000	1.00	0.00
LYS86	HG2	1.00	0.000	1.00	0.00
LYS86	HG3	1.00	0.000	1.00	0.00
LYS86	HD2	1.00	0.000	1.00	0.00
LYS86	HD3	1.00	0.000	1.00	0.00
LYS86	HE2	1.00	0.000	1.00	0.00
LYS86	HE3	1.00	0.000	1.00	0.00

**3.86.16 Detailed Probabilities of LYS86H:**

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
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	0.000	1.00	0.00
LEU85	HB2	1.00	0.000	1.00	0.00
LEU85	HB3	1.00	0.000	1.00	0.00
LEU85	HG	0.98	0.000	1.00	0.00
LEU85	H	1.00	0.000	1.00	0.00
LEU85	HD11	0.52	0.000	1.00	0.00
LEU85	HD21	0.59	0.000	1.00	0.00
LYS86	HA	1.00	0.000	1.00	0.00
LYS86	HB2	1.00	0.000	1.00	0.00
LYS86	HB3	1.00	0.000	1.00	0.00
LYS86	HG2	1.00	0.000	1.00	0.00
LYS86	HG3	1.00	0.000	1.00	0.00
LYS86	H	1.00	0.000	1.00	0.00
LYS86	HD2	0.88	0.000	1.00	0.00
LYS86	HD3	0.87	0.000	1.00	0.00
PRO87	HD2	0.99	0.009	1.00	0.00
PRO87	HD3	0.99	0.009	1.00	0.00

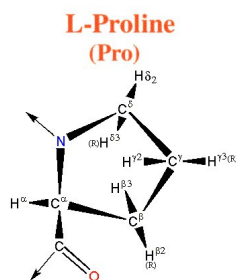


Figure 77: Image from the BMRB

**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
C	179.579	175.173	13.901	0.000	0.000
CA 3.87.1	66.718	62.931	15.301	0.818	1.000
CB 3.87.2	30.461	33.632	13.629	1.000	1.000
CG 3.87.3	28.529	28.412	13.801	1.000	1.000
CD 3.87.4	50.193	49.797	3.175	1.000	1.000
N	NA	—	—	0.000	0.000
HA 3.87.5	4.287	4.332	0.427	0.800	1.000
HB2 3.87.6	1.914	2.099	0.501	0.890	1.000
HB3 3.87.7	2.360	2.052	0.596	1.000	1.000
HG2 3.87.8	1.970	1.927	0.364	1.000	1.000
HG3 3.87.9	2.184	1.907	0.417	1.000	1.000
HD2 3.87.10	3.657	3.640	0.682	0.933	1.000
HD3 3.87.11	3.449	3.558	0.522	0.909	1.000

**3.87.1 Detailed Probabilities of PRO87CA:**

**Overall probability:** 0.818  
**Overall confidence:** 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS86	0.50	1.00
PRO87	1.00	1.00
ASP88	0.50	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	0.147	0.00	0.00
LYS86	HB3	0.80	0.008	1.00	0.00
PRO87	HA	1.00	0.000	1.00	0.00
PRO87	HB2	1.00	0.000	1.00	0.00
PRO87	HB3	1.00	0.000	1.00	0.00
PRO87	HG2	1.00	0.000	1.00	0.00
PRO87	HG3	1.00	0.000	1.00	0.00
PRO87	HD2	1.00	0.000	1.00	0.00
PRO87	HD3	1.00	0.000	1.00	0.00
ASP88	HA	1.00	0.330	0.00	0.00
ASP88	H	1.00	0.000	1.00	0.00

**3.87.2 Detailed Probabilities of PRO87CB:**

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

**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**

## 3.87 PRO(87)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PRO87	HA	1.00	0.000	1.00	0.00
PRO87	HB2	1.00	0.000	1.00	0.00
PRO87	HB3	1.00	0.000	1.00	0.00
PRO87	HG2	1.00	0.000	1.00	0.00
PRO87	HG3	1.00	0.000	1.00	0.00
PRO87	HD2	1.00	0.000	1.00	0.00
PRO87	HD3	1.00	0.000	1.00	0.00
ASP88	H	1.00	0.000	1.00	0.00

## 3.87.3 Detailed Probabilities of PRO87CG:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
PRO87	1.00	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	0.000	1.00	0.00
PRO87	HB2	1.00	0.000	1.00	0.00
PRO87	HB3	1.00	0.000	1.00	0.00
PRO87	HG2	1.00	0.000	1.00	0.00
PRO87	HG3	1.00	0.000	1.00	0.00
PRO87	HD2	1.00	0.000	1.00	0.00
PRO87	HD3	1.00	0.000	1.00	0.00

## 3.87.4 Detailed Probabilities of PRO87CD:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
LYS86	1.00	1.00
PRO87	1.00	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	0.00
LYS86	HB2	1.00	0.020	1.00	0.00
LYS86	HB3	1.00	0.008	1.00	0.00
LYS86	H	0.99	0.009	1.00	0.00
LYS86	HG2	0.79	0.007	1.00	0.00
LYS86	HG3	0.78	0.008	1.00	0.00
PRO87	HA	1.00	0.000	1.00	0.00
PRO87	HB2	1.00	0.000	1.00	0.00
PRO87	HB3	1.00	0.000	1.00	0.00
PRO87	HG2	1.00	0.000	1.00	0.00
PRO87	HG3	1.00	0.000	1.00	0.00
PRO87	HD2	1.00	0.000	1.00	0.00
PRO87	HD3	1.00	0.000	1.00	0.00

**3.87.5 Detailed Probabilities of PRO87HA:**

Overall probability: 0.800

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS86	0.00	1.00
PRO87	1.00	1.00
ASP88	0.50	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	0.483	0.00	0.00
PRO87	HA	1.00	0.000	1.00	0.00
PRO87	HB2	1.00	0.000	1.00	0.00
PRO87	HB3	1.00	0.000	1.00	0.00
PRO87	HG2	1.00	0.000	1.00	0.00
PRO87	HG3	1.00	0.000	1.00	0.00
PRO87	HD2	1.00	0.000	1.00	0.00
PRO87	HD3	1.00	0.000	1.00	0.00
ASP88	HA	1.00	0.330	0.00	0.00
ASP88	H	1.00	0.000	1.00	0.00

**3.87.6 Detailed Probabilities of PRO87HB2:**

Overall probability: 0.890

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO87	1.00	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	0.000	1.00	0.00
PRO87	HB2	1.00	0.000	1.00	0.00
PRO87	HB3	1.00	0.000	1.00	0.00
PRO87	HG2	1.00	0.000	1.00	0.00
PRO87	HG3	1.00	0.000	1.00	0.00
PRO87	HD2	1.00	0.000	1.00	0.00
PRO87	HD3	1.00	0.000	1.00	0.00
ASP88	HA	0.99	0.353	0.01	0.00
ASP88	H	1.00	0.000	1.00	0.00

**3.87.7 Detailed Probabilities of PRO87HB3:**

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

**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	0.000	1.00	0.00
PRO87	HB2	1.00	0.000	1.00	0.00
PRO87	HB3	1.00	0.000	1.00	0.00
PRO87	HG2	1.00	0.000	1.00	0.00
PRO87	HG3	1.00	0.000	1.00	0.00
PRO87	HD2	1.00	0.000	1.00	0.00
PRO87	HD3	1.00	0.000	1.00	0.00
ASP88	H	1.00	0.000	1.00	0.00

**3.87.8 Detailed Probabilities of PRO87HG2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO87	1.00	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	0.000	1.00	0.00
PRO87	HB2	1.00	0.000	1.00	0.00
PRO87	HB3	1.00	0.000	1.00	0.00
PRO87	HG2	1.00	0.000	1.00	0.00
PRO87	HG3	1.00	0.000	1.00	0.00
PRO87	HD2	1.00	0.000	1.00	0.00
PRO87	HD3	1.00	0.000	1.00	0.00

**3.87.9 Detailed Probabilities of PRO87HG3:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO87	1.00	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	0.000	1.00	0.00
PRO87	HB2	1.00	0.000	1.00	0.00
PRO87	HB3	1.00	0.000	1.00	0.00
PRO87	HG2	1.00	0.000	1.00	0.00
PRO87	HG3	1.00	0.000	1.00	0.00
PRO87	HD2	1.00	0.000	1.00	0.00
PRO87	HD3	1.00	0.000	1.00	0.00

**3.87.10 Detailed Probabilities of PRO87HD2:**

Overall probability: 0.933

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS86	0.88	1.00
PRO87	1.00	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	0.147	0.00	0.00
LYS86	HB2	0.99	0.005	1.00	0.00
LYS86	HB3	0.99	0.007	1.00	0.00
LYS86	H	0.99	0.015	1.00	0.00
LYS86	HG2	0.93	0.028	1.00	0.00
LYS86	HG3	0.92	0.029	1.00	0.00
LYS86	HD2	0.66	0.008	1.00	0.00
LYS86	HD3	0.66	0.008	1.00	0.00
PRO87	HA	1.00	0.000	1.00	0.00
PRO87	HB2	1.00	0.000	1.00	0.00
PRO87	HB3	1.00	0.000	1.00	0.00
PRO87	HG2	1.00	0.000	1.00	0.00
PRO87	HG3	1.00	0.000	1.00	0.00
PRO87	HD2	1.00	0.000	1.00	0.00
PRO87	HD3	1.00	0.000	1.00	0.00

**3.87.11 Detailed Probabilities of PRO87HD3:**

Overall probability: 0.909

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LYS86	0.75	1.00
PRO87	1.00	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	0.248	0.00	0.00
LYS86	HB2	1.00	0.003	1.00	0.00
LYS86	HB3	1.00	0.003	1.00	0.00
LYS86	H	0.99	0.003	1.00	0.00
PRO87	HA	1.00	0.000	1.00	0.00
PRO87	HB2	1.00	0.000	1.00	0.00
PRO87	HB3	1.00	0.000	1.00	0.00
PRO87	HG2	1.00	0.000	1.00	0.00
PRO87	HG3	1.00	0.000	1.00	0.00
PRO87	HD2	1.00	0.000	1.00	0.00
PRO87	HD3	1.00	0.000	1.00	0.00

**3.88 ASP(88)**

Figure 78: Image from the BMRB

Residue probability: 0.893

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	0.627	0.889
CB 3.88.2	40.867	40.949	3.070	1.000	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	0.627	0.889
HB2 3.88.5	2.679	2.708	0.282	1.000	0.833
HB3 3.88.6	2.591	2.654	0.285	1.000	0.833
H 3.88.7	7.457	8.304	1.027	1.000	1.000

**3.88.1 Detailed Probabilities of ASP88CA:**

Overall probability: 0.627

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO87	0.01	1.00
ASP88	1.00	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	0.353	0.01	0.00
ASP88	HA	1.00	0.000	1.00	0.00
ASP88	HB2	1.00	0.000	1.00	0.00
ASP88	HB3	1.00	0.000	1.00	0.00
ASP88	H	1.00	0.000	1.00	0.00
ILE89	HA	1.00	0.183	0.00	0.00
ILE89	H	1.00	0.000	1.00	0.00

**3.88.2 Detailed Probabilities of ASP88CB:**

Overall probability: 1.000

Overall confidence: 0.833

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASP88	1.00	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	0.000	1.00	0.00
ASP88	HB2	1.00	0.000	1.00	0.00
ASP88	HB3	1.00	0.000	1.00	0.00
ASP88	H	1.00	0.000	1.00	0.00
ILE89	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
PRO87	HB2	1.00	0.000	1.00	0.00
PRO87	HB3	1.00	0.000	1.00	0.00
PRO87	HG2	0.95	0.000	1.00	0.00
PRO87	HG3	0.87	0.000	1.00	0.00
PRO87	HD2	0.82	0.000	1.00	0.00
PRO87	HD3	0.72	0.000	1.00	0.00
ASP88	HA	1.00	0.000	1.00	0.00
ASP88	HB2	1.00	0.000	1.00	0.00
ASP88	HB3	1.00	0.000	1.00	0.00
ASP88	H	1.00	0.000	1.00	0.00
ILE89	H	1.00	0.000	1.00	0.00
ILE89	HB	0.52	0.014	1.00	0.00
ILE89	HG13	0.56	0.013	1.00	0.00

**3.88.4 Detailed Probabilities of ASP88HA:**

Overall probability: 0.627

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO87	0.01	1.00
ASP88	1.00	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	0.198	0.01	0.00
ASP88	HA	1.00	0.000	1.00	0.00
ASP88	HB2	1.00	0.000	1.00	0.00
ASP88	HB3	1.00	0.000	1.00	0.00
ASP88	H	1.00	0.000	1.00	0.00
ILE89	HA	1.00	0.417	0.00	0.00
ILE89	H	1.00	0.000	1.00	0.00

**3.88.5 Detailed Probabilities of ASP88HB2:**

Overall probability: 1.000

Overall confidence: 0.833

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASP88	1.00	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	0.000	1.00	0.00
ASP88	HB2	1.00	0.000	1.00	0.00
ASP88	HB3	1.00	0.000	1.00	0.00
ASP88	H	1.00	0.000	1.00	0.00
ILE89	H	1.00	0.000	1.00	0.00

**3.88.6 Detailed Probabilities of ASP88HB3:**

Overall probability: 1.000

Overall confidence: 0.833

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASP88	1.00	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	0.000	1.00	0.00
ASP88	HB2	1.00	0.000	1.00	0.00
ASP88	HB3	1.00	0.000	1.00	0.00
ASP88	H	1.00	0.000	1.00	0.00
ILE89	H	1.00	0.000	1.00	0.00

**3.88.7 Detailed Probabilities of ASP88H:**

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	0.000	1.00	0.00
PRO87	HB2	1.00	0.000	1.00	0.00
PRO87	HB3	1.00	0.000	1.00	0.00
PRO87	HG2	0.95	0.000	1.00	0.00
PRO87	HG3	0.87	0.000	1.00	0.00
PRO87	HD2	0.82	0.000	1.00	0.00
PRO87	HD3	0.72	0.000	1.00	0.00
ASP88	HA	1.00	0.000	1.00	0.00
ASP88	HB2	1.00	0.000	1.00	0.00
ASP88	HB3	1.00	0.000	1.00	0.00
ASP88	H	1.00	0.000	1.00	0.00
ILE89	H	1.00	0.000	1.00	0.00

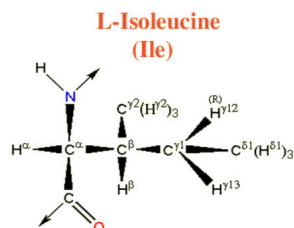


Figure 79: Image from the BMRB

Residue probability: 0.969  
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	0.800	1.000
CB 3.89.2	37.729	38.702	3.945	1.000	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	1.000	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	0.800	1.000
HB 3.89.8	1.452	1.776	0.310	1.000	1.000
HG12 3.89.9	1.830	1.271	0.411	1.000	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	1.000	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: 0.800  
Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASP88	0.00	1.00
ILE89	1.00	1.00
TYR90	0.50	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	0.417	0.00	0.00
ILE89	HA	1.00	0.000	1.00	0.00
ILE89	HB	1.00	0.000	1.00	0.00
ILE89	HG12	1.00	0.000	1.00	0.00
ILE89	HG13	1.00	0.000	1.00	0.00
ILE89	HG21	1.00	0.000	1.00	0.00
ILE89	HD11	0.97	0.000	1.00	0.00
ILE89	H	1.00	0.000	1.00	0.00
TYR90	HA	1.00	0.223	0.00	0.00
TYR90	H	1.00	0.000	1.00	0.00

**3.89.2 Detailed Probabilities of ILE89CB:**

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
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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE89	HA	1.00	0.000	1.00	0.00
ILE89	HB	1.00	0.000	1.00	0.00
ILE89	HG12	1.00	0.000	1.00	0.00
ILE89	HG13	1.00	0.000	1.00	0.00
ILE89	HG21	1.00	0.000	1.00	0.00
ILE89	HD11	1.00	0.000	1.00	0.00
ILE89	H	1.00	0.000	1.00	0.00
TYR90	H	1.00	0.000	1.00	0.00

## 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
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	0.00
ILE89	HB	1.00	0.000	1.00	0.00
ILE89	HG12	1.00	0.000	1.00	0.00
ILE89	HG13	1.00	0.000	1.00	0.00
ILE89	HG21	1.00	0.000	1.00	0.00
ILE89	HD11	1.00	0.000	1.00	0.00
ILE89	H	1.00	0.000	1.00	0.00
TYR90	H	0.99	0.000	1.00	0.00

## 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	0.000	1.00	0.00
ILE89	HB	1.00	0.000	1.00	0.00
ILE89	HG12	1.00	0.000	1.00	0.00
ILE89	HG13	1.00	0.000	1.00	0.00
ILE89	HG21	1.00	0.000	1.00	0.00
ILE89	HD11	0.99	0.000	1.00	0.00
ILE89	H	1.00	0.000	1.00	0.00
TYR90	H	0.98	0.000	1.00	0.00
TYR90	HA	0.66	0.018	1.00	0.00

**3.89.5 Detailed Probabilities of ILE89CD1:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE89	1.00	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	0.000	1.00	0.00
ILE89	HB	1.00	0.000	1.00	0.00
ILE89	HG12	1.00	0.000	1.00	0.00
ILE89	HG13	1.00	0.000	1.00	0.00
ILE89	HG21	0.99	0.000	1.00	0.00
ILE89	HD11	1.00	0.000	1.00	0.00
ILE89	H	0.94	0.000	1.00	0.00

**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	0.000	1.00	0.00
ASP88	HB2	1.00	0.000	1.00	0.00
ASP88	HB3	1.00	0.000	1.00	0.00
ASP88	H	1.00	0.000	1.00	0.00
ILE89	HA	1.00	0.000	1.00	0.00
ILE89	HB	1.00	0.000	1.00	0.00
ILE89	HG12	1.00	0.000	1.00	0.00
ILE89	HG13	1.00	0.000	1.00	0.00
ILE89	HG21	1.00	0.000	1.00	0.00
ILE89	H	1.00	0.000	1.00	0.00
ILE89	HD11	0.94	0.000	1.00	0.00
TYR90	H	1.00	0.000	1.00	0.00

**3.89.7 Detailed Probabilities of ILE89HA:**

Overall probability: 0.800

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASP88	0.00	1.00
ILE89	1.00	1.00
TYR90	0.50	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	0.183	0.00	0.00
ILE89	HA	1.00	0.000	1.00	0.00
ILE89	HB	1.00	0.000	1.00	0.00
ILE89	HG12	1.00	0.000	1.00	0.00
ILE89	HG13	1.00	0.000	1.00	0.00
ILE89	HG21	1.00	0.000	1.00	0.00
ILE89	HD11	0.97	0.000	1.00	0.00
ILE89	H	1.00	0.000	1.00	0.00
TYR90	HA	1.00	0.050	0.00	0.00
TYR90	H	1.00	0.000	1.00	0.00

**3.89.8 Detailed Probabilities of ILE89HB:**

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
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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE89	HA	1.00	0.000	1.00	0.00
ILE89	HB	1.00	0.000	1.00	0.00
ILE89	HG12	1.00	0.000	1.00	0.00
ILE89	HG13	1.00	0.000	1.00	0.00
ILE89	HG21	1.00	0.000	1.00	0.00
ILE89	HD11	1.00	0.000	1.00	0.00
ILE89	H	1.00	0.000	1.00	0.00
TYR90	H	1.00	0.000	1.00	0.00
TYR90	HA	0.90	0.014	1.00	0.00

## 3.89.9 Detailed Probabilities of ILE89HG12:

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
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	0.00
ILE89	HB	1.00	0.000	1.00	0.00
ILE89	HG12	1.00	0.000	1.00	0.00
ILE89	HG13	1.00	0.000	1.00	0.00
ILE89	HG21	1.00	0.000	1.00	0.00
ILE89	HD11	1.00	0.000	1.00	0.00
ILE89	H	1.00	0.000	1.00	0.00
TYR90	H	0.99	0.000	1.00	0.00

## 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	0.000	1.00	0.00
ILE89	HB	1.00	0.000	1.00	0.00
ILE89	HG12	1.00	0.000	1.00	0.00
ILE89	HG13	1.00	0.000	1.00	0.00
ILE89	HG21	1.00	0.000	1.00	0.00
ILE89	HD11	1.00	0.000	1.00	0.00
ILE89	H	1.00	0.000	1.00	0.00
TYR90	H	0.96	0.000	1.00	0.00

**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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE89	HA	1.00	0.000	1.00	0.00
ILE89	HB	1.00	0.000	1.00	0.00
ILE89	HG12	1.00	0.000	1.00	0.00
ILE89	HG13	1.00	0.000	1.00	0.00
ILE89	HG21	1.00	0.000	1.00	0.00
ILE89	HD11	0.99	0.000	1.00	0.00
ILE89	H	1.00	0.000	1.00	0.00
TYR90	H	0.98	0.000	1.00	0.00
TYR90	HA	0.66	0.002	1.00	0.00

**3.89.12 Detailed Probabilities of ILE89HD11:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE89	1.00	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	0.000	1.00	0.00
ILE89	HB	1.00	0.000	1.00	0.00
ILE89	HG12	1.00	0.000	1.00	0.00
ILE89	HG13	1.00	0.000	1.00	0.00
ILE89	HG21	0.99	0.000	1.00	0.00
ILE89	HD11	1.00	0.000	1.00	0.00
ILE89	H	0.94	0.000	1.00	0.00

**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	0.000	1.00	0.00
ASP88	HB2	1.00	0.000	1.00	0.00
ASP88	HB3	1.00	0.000	1.00	0.00
ASP88	H	1.00	0.000	1.00	0.00
ILE89	HA	1.00	0.000	1.00	0.00
ILE89	HB	1.00	0.000	1.00	0.00
ILE89	HG12	1.00	0.000	1.00	0.00
ILE89	HG13	1.00	0.000	1.00	0.00
ILE89	HG21	1.00	0.000	1.00	0.00
ILE89	H	1.00	0.000	1.00	0.00
ILE89	HD11	0.94	0.000	1.00	0.00
TYR90	H	1.00	0.000	1.00	0.00

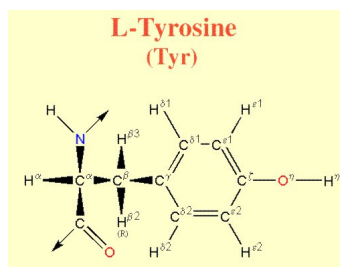


Figure 80: Image from the BMRB

Residue probability: 0.977  
 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	1.000	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	1.000	1.000
HA 3.90.8	3.977	4.610	0.592	0.818	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	0.050	0.00	0.00
ILE89	HB	0.90	0.014	1.00	0.00
ILE89	HG21	0.68	0.002	1.00	0.00
TYR90	HA	1.00	0.000	1.00	0.00
TYR90	HB2	1.00	0.000	1.00	0.00
TYR90	HB3	1.00	0.000	1.00	0.00
TYR90	HD1	1.00	0.002	1.00	0.00
TYR90	HD2	1.00	0.002	1.00	0.00
TYR90	H	1.00	0.000	1.00	0.00
TYR90	HE1	0.75	0.003	1.00	0.00
ALA91	HA	1.00	0.062	0.00	0.00
ALA91	H	1.00	0.000	1.00	0.00

**3.90.2 Detailed Probabilities of TYR90CB:**

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**

## 3.90 TYR(90)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR90	HA	1.00	0.000	1.00	0.00
TYR90	HB2	1.00	0.000	1.00	0.00
TYR90	HB3	1.00	0.000	1.00	0.00
TYR90	HD1	1.00	0.002	1.00	0.00
TYR90	HD2	1.00	0.002	1.00	0.00
TYR90	HE2	1.00	0.003	1.00	0.00
TYR90	H	1.00	0.000	1.00	0.00
TYR90	HE1	0.89	0.003	1.00	0.00
ALA91	H	1.00	0.000	1.00	0.00
ALA91	HA	0.66	0.014	1.00	0.00

## 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	0.000	1.00	0.00
TYR90	HB2	1.00	0.000	1.00	0.00
TYR90	HB3	1.00	0.000	1.00	0.00
TYR90	HD1	1.00	0.001	1.00	0.00
TYR90	HD2	1.00	0.001	1.00	0.00
TYR90	HE1	1.00	0.003	1.00	0.00
TYR90	HE2	1.00	0.003	1.00	0.00
TYR90	H	1.00	0.003	1.00	0.00

## 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	0.000	1.00	0.00
TYR90	HB2	1.00	0.000	1.00	0.00
TYR90	HB3	1.00	0.000	1.00	0.00
TYR90	HD1	1.00	0.001	1.00	0.00
TYR90	HD2	1.00	0.001	1.00	0.00
TYR90	HE1	1.00	0.003	1.00	0.00
TYR90	HE2	1.00	0.003	1.00	0.00
TYR90	H	0.98	0.003	1.00	0.00

**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	0.001	1.00	0.00
TYR90	HD2	1.00	0.001	1.00	0.00
TYR90	HE1	1.00	0.003	1.00	0.00
TYR90	HE2	1.00	0.003	1.00	0.00
TYR90	HA	0.75	0.000	1.00	0.00
TYR90	HB2	0.89	0.000	1.00	0.00
TYR90	HB3	0.88	0.000	1.00	0.00

**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	0.000	1.00	0.00
TYR90	HB3	1.00	0.000	1.00	0.00
TYR90	HD1	1.00	0.001	1.00	0.00
TYR90	HD2	1.00	0.001	1.00	0.00
TYR90	HE1	1.00	0.003	1.00	0.00
TYR90	HE2	1.00	0.003	1.00	0.00

**3.90.7 Detailed Probabilities of TYR90N:**

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	0.000	1.00	0.00
ILE89	HB	1.00	0.000	1.00	0.00
ILE89	HG12	0.99	0.000	1.00	0.00
ILE89	HG13	0.96	0.000	1.00	0.00
ILE89	HG21	0.98	0.000	1.00	0.00
ILE89	H	1.00	0.000	1.00	0.00
TYR90	HA	1.00	0.000	1.00	0.00
TYR90	HB2	1.00	0.000	1.00	0.00
TYR90	HB3	1.00	0.000	1.00	0.00
TYR90	HD1	1.00	0.002	1.00	0.00
TYR90	HD2	0.98	0.002	1.00	0.00
TYR90	H	1.00	0.000	1.00	0.00
ALA91	H	1.00	0.000	1.00	0.00

**3.90.8 Detailed Probabilities of TYR90HA:**

Overall probability: 0.818

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE89	0.50	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	0.223	0.00	0.00
ILE89	HG21	0.68	0.018	1.00	0.00
TYR90	HA	1.00	0.000	1.00	0.00
TYR90	HB2	1.00	0.000	1.00	0.00
TYR90	HB3	1.00	0.000	1.00	0.00
TYR90	HD1	1.00	0.000	1.00	0.00
TYR90	HD2	1.00	0.000	1.00	0.00
TYR90	H	1.00	0.000	1.00	0.00
TYR90	HE1	0.75	0.000	1.00	0.00
ALA91	HA	1.00	0.062	0.00	0.00
ALA91	H	1.00	0.000	1.00	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	0.000	1.00	0.00
TYR90	HB2	1.00	0.000	1.00	0.00
TYR90	HB3	1.00	0.000	1.00	0.00
TYR90	HD1	1.00	0.000	1.00	0.00
TYR90	HD2	1.00	0.000	1.00	0.00
TYR90	HE2	1.00	0.000	1.00	0.00
TYR90	H	1.00	0.000	1.00	0.00
TYR90	HE1	0.89	0.000	1.00	0.00
ALA91	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
TYR90	HB2	1.00	0.000	1.00	0.00
TYR90	HB3	1.00	0.000	1.00	0.00
TYR90	HD1	1.00	0.000	1.00	0.00
TYR90	HD2	1.00	0.000	1.00	0.00
TYR90	HE2	1.00	0.000	1.00	0.00
TYR90	H	1.00	0.000	1.00	0.00
TYR90	HE1	0.88	0.000	1.00	0.00
ALA91	H	1.00	0.000	1.00	0.00

**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	0.002	1.00	0.00
TYR90	HB2	1.00	0.002	1.00	0.00
TYR90	HB3	1.00	0.002	1.00	0.00
TYR90	HD1	1.00	0.001	1.00	0.00
TYR90	HD2	1.00	0.001	1.00	0.00
TYR90	HE1	1.00	0.001	1.00	0.00
TYR90	HE2	1.00	0.001	1.00	0.00
TYR90	H	1.00	0.002	1.00	0.00

**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	0.002	1.00	0.00
TYR90	HB2	1.00	0.002	1.00	0.00
TYR90	HB3	1.00	0.002	1.00	0.00
TYR90	HD1	1.00	0.001	1.00	0.00
TYR90	HD2	1.00	0.001	1.00	0.00
TYR90	HE1	1.00	0.001	1.00	0.00
TYR90	HE2	1.00	0.001	1.00	0.00
TYR90	H	0.98	0.002	1.00	0.00

**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	0.003	1.00	0.00
TYR90	HD2	1.00	0.003	1.00	0.00
TYR90	HE1	1.00	0.003	1.00	0.00
TYR90	HE2	1.00	0.003	1.00	0.00
TYR90	HA	0.75	0.003	1.00	0.00
TYR90	HB2	0.89	0.003	1.00	0.00
TYR90	HB3	0.88	0.003	1.00	0.00

**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	0.003	1.00	0.00
TYR90	HB3	1.00	0.003	1.00	0.00
TYR90	HD1	1.00	0.003	1.00	0.00
TYR90	HD2	1.00	0.003	1.00	0.00
TYR90	HE1	1.00	0.003	1.00	0.00
TYR90	HE2	1.00	0.003	1.00	0.00

**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	0.000	1.00	0.00
ILE89	HB	1.00	0.000	1.00	0.00
ILE89	HG12	0.99	0.000	1.00	0.00
ILE89	HG13	0.96	0.000	1.00	0.00
ILE89	HG21	0.98	0.000	1.00	0.00
ILE89	H	1.00	0.000	1.00	0.00
TYR90	HA	1.00	0.000	1.00	0.00
TYR90	HB2	1.00	0.000	1.00	0.00
TYR90	HB3	1.00	0.000	1.00	0.00
TYR90	HD1	1.00	0.003	1.00	0.00
TYR90	HD2	0.98	0.003	1.00	0.00
TYR90	H	1.00	0.000	1.00	0.00
ALA91	H	1.00	0.000	1.00	0.00

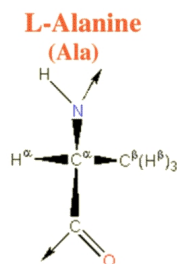
**3.91 ALA(91)**

Figure 81: Image from the BMRB

Residue probability: 0.903

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	0.667	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	1.000	1.000
HA 3.91.4	4.039	4.254	0.459	0.750	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: 0.667

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
TYR90	0.00	1.00
ALA91	1.00	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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR90	HA	1.00	0.062	0.00	0.00
ALA91	HA	1.00	0.000	1.00	0.00
ALA91	HB1	1.00	0.000	1.00	0.00
ALA91	H	1.00	0.000	1.00	0.00
THR92	HA	1.00	0.062	0.00	0.00
THR92	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ALA91	HB1	1.00	0.000	1.00	0.00
ALA91	H	1.00	0.000	1.00	0.00
THR92	H	1.00	0.000	1.00	0.00

**3.91.3 Detailed Probabilities of ALA91N:**

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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR90	HA	1.00	0.000	1.00	0.00
TYR90	HB2	1.00	0.000	1.00	0.00
TYR90	HB3	1.00	0.000	1.00	0.00
TYR90	H	1.00	0.000	1.00	0.00
TYR90	HD1	0.79	0.001	1.00	0.00
TYR90	HD2	0.68	0.001	1.00	0.00
ALA91	HA	1.00	0.000	1.00	0.00
ALA91	HB1	1.00	0.000	1.00	0.00
ALA91	H	1.00	0.000	1.00	0.00
THR92	H	1.00	0.010	1.00	0.00
THR92	HA	0.85	0.000	1.00	0.00

## 3.91.4 Detailed Probabilities of ALA91HA:

Overall probability: 0.750

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
TYR90	0.67	1.00
ALA91	1.00	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

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR90	HA	1.00	0.062	0.00	0.00
TYR90	HB2	0.66	0.014	1.00	0.00
TYR90	HB3	0.85	0.014	1.00	0.00
ALA91	HA	1.00	0.000	1.00	0.00
ALA91	HB1	1.00	0.000	1.00	0.00
ALA91	H	1.00	0.000	1.00	0.00
THR92	HA	1.00	0.062	0.00	0.00
THR92	H	1.00	0.000	1.00	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	0.000	1.00	0.00
ALA91	HB1	1.00	0.000	1.00	0.00
ALA91	H	1.00	0.000	1.00	0.00
THR92	H	1.00	0.000	1.00	0.00
THR92	HA	0.71	0.025	1.00	0.00

**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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR90	HA	1.00	0.000	1.00	0.00
TYR90	HB2	1.00	0.000	1.00	0.00
TYR90	HB3	1.00	0.000	1.00	0.00
TYR90	H	1.00	0.000	1.00	0.00
TYR90	HD1	0.79	0.000	1.00	0.00
TYR90	HD2	0.68	0.000	1.00	0.00
ALA91	HA	1.00	0.000	1.00	0.00
ALA91	HB1	1.00	0.000	1.00	0.00
ALA91	H	1.00	0.000	1.00	0.00
THR92	H	1.00	0.010	1.00	0.00
THR92	HA	0.85	0.010	1.00	0.00

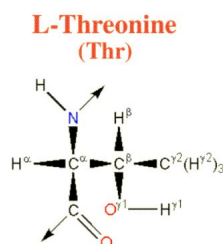
**3.92 THR(92)**

Figure 82: Image from the BMRB

Residue probability: 0.944

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	0.778	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	1.000	0.833
N 3.92.4	114.461	115.370	5.913	1.000	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	1.000	0.833
H 3.92.8	7.937	8.272	1.597	1.000	0.889
HG1	NA	—	—	0.000	0.000

**3.92.1 Detailed Probabilities of THR92CA:**

Overall probability: 0.778

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ALA91	0.67	1.00
THR92	1.00	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	0.062	0.00	0.00
ALA91	HB1	0.67	0.025	1.00	0.00
ALA91	H	0.85	0.010	1.00	0.00
THR92	HA	1.00	0.000	1.00	0.00
THR92	HB	1.00	0.000	1.00	0.00
THR92	HG21	1.00	0.000	1.00	0.00
THR92	H	1.00	0.000	1.00	0.00
ILE93	HA	1.00	0.454	0.00	0.00
ILE93	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
THR92	HB	1.00	0.000	1.00	0.00
THR92	HG21	1.00	0.000	1.00	0.00
THR92	H	1.00	0.000	1.00	0.00
ILE93	H	1.00	0.000	1.00	0.00

**3.92.3 Detailed Probabilities of THR92CG2:**

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
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	0.000	1.00	0.00
THR92	HB	1.00	0.000	1.00	0.00
THR92	HG21	1.00	0.000	1.00	0.00
THR92	H	1.00	0.000	1.00	0.00
ILE93	H	0.98	0.000	1.00	0.00

**3.92.4 Detailed Probabilities of THR92N:**

Overall probability: 1.000

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ALA91	1.00	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	0.000	1.00	0.00
ALA91	HB1	1.00	0.000	1.00	0.00
ALA91	H	1.00	0.010	1.00	0.00
THR92	HA	1.00	0.000	1.00	0.00
THR92	HB	1.00	0.000	1.00	0.00
THR92	HG21	1.00	0.000	1.00	0.00
THR92	H	1.00	0.000	1.00	0.00
ILE93	H	1.00	0.000	1.00	0.00

**3.92.5 Detailed Probabilities of THR92HA:**

Overall probability: 0.778

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ALA91	0.50	1.00
THR92	1.00	0.80
ILE93	0.67	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	0.062	0.00	0.00
ALA91	H	0.85	0.000	1.00	0.00
THR92	HA	1.00	0.000	1.00	0.00
THR92	HB	1.00	0.000	1.00	0.00
THR92	HG21	1.00	0.000	1.00	0.00
THR92	H	1.00	0.000	1.00	0.00
ILE93	HA	1.00	0.454	0.00	0.00
ILE93	H	1.00	0.000	1.00	0.00
ILE93	HB	0.59	0.000	1.00	0.00

**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	0.000	1.00	0.00
THR92	HB	1.00	0.000	1.00	0.00
THR92	HG21	1.00	0.000	1.00	0.00
THR92	H	1.00	0.000	1.00	0.00
ILE93	H	1.00	0.000	1.00	0.00

**3.92.7 Detailed Probabilities of THR92HG21:**

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
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	0.000	1.00	0.00
THR92	HB	1.00	0.000	1.00	0.00
THR92	HG21	1.00	0.000	1.00	0.00
THR92	H	1.00	0.000	1.00	0.00
ILE93	H	0.98	0.000	1.00	0.00
ILE93	HA	0.50	0.008	1.00	0.00

**3.92.8 Detailed Probabilities of THR92H:**

Overall probability: 1.000

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ALA91	1.00	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	0.000	1.00	0.00
ALA91	HB1	1.00	0.000	1.00	0.00
ALA91	H	1.00	0.010	1.00	0.00
THR92	HA	1.00	0.000	1.00	0.00
THR92	HB	1.00	0.000	1.00	0.00
THR92	HG21	1.00	0.000	1.00	0.00
THR92	H	1.00	0.000	1.00	0.00
ILE93	H	1.00	0.000	1.00	0.00

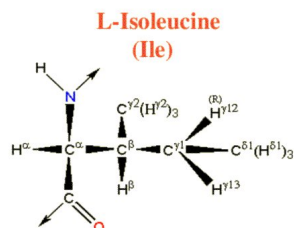


Figure 83: Image from the BMRB

Residue probability: 0.971  
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	0.818	1.000
CB 3.93.2	37.978	38.702	3.945	1.000	1.000
CG1 3.93.3	29.576	27.785	2.037	1.000	1.000
CG2 3.93.4	17.769	17.574	1.928	1.000	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	0.800	1.000
HB 3.93.8	1.852	1.776	0.310	1.000	1.000
HG12 3.93.9	0.626	1.271	0.411	1.000	1.000
HG13 3.93.10	1.947	1.186	0.426	1.000	1.000
HG2 3.93.11	0.884	0.762	0.283	1.000	1.000
HD1 3.93.12	0.507	0.668	0.293	1.000	1.000
H 3.93.13	8.253	8.301	0.685	1.000	0.917

**3.93.1 Detailed Probabilities of ILE93CA:**

Overall probability: 0.818  
Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR92	0.50	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	0.454	0.00	0.00
THR92	HG21	0.52	0.008	1.00	0.00
ILE93	HA	1.00	0.000	1.00	0.00
ILE93	HB	1.00	0.000	1.00	0.00
ILE93	HG12	1.00	0.000	1.00	0.00
ILE93	HG13	1.00	0.000	1.00	0.00
ILE93	HG21	1.00	0.000	1.00	0.00
ILE93	HD11	0.97	0.000	1.00	0.00
ILE93	H	1.00	0.000	1.00	0.00
MET94	HA	1.00	0.756	0.00	0.00
MET94	H	1.00	0.000	1.00	0.00

**3.93.2 Detailed Probabilities of ILE93CB:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE93	1.00	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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE93	HA	1.00	0.000	1.00	0.00
ILE93	HB	1.00	0.000	1.00	0.00
ILE93	HG12	1.00	0.000	1.00	0.00
ILE93	HG13	1.00	0.000	1.00	0.00
ILE93	HG21	1.00	0.000	1.00	0.00
ILE93	HD11	1.00	0.000	1.00	0.00
ILE93	H	1.00	0.000	1.00	0.00
MET94	H	1.00	0.000	1.00	0.00

#### 3.93.3 Detailed Probabilities of ILE93CG1:

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	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	0.000	1.00	0.00
ILE93	HB	1.00	0.000	1.00	0.00
ILE93	HG12	1.00	0.000	1.00	0.00
ILE93	HG13	1.00	0.000	1.00	0.00
ILE93	HG21	1.00	0.000	1.00	0.00
ILE93	HD11	1.00	0.000	1.00	0.00
ILE93	H	1.00	0.000	1.00	0.00

#### 3.93.4 Detailed Probabilities of ILE93CG2:

Overall probability: 1.000

Overall confidence: 1.000

##### Inter- and intra-residue probability

Residue	Probability	Confidence
ILE93	1.00	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	0.000	1.00	0.00
ILE93	HB	1.00	0.000	1.00	0.00
ILE93	HG12	1.00	0.000	1.00	0.00
ILE93	HG13	1.00	0.000	1.00	0.00
ILE93	HG21	1.00	0.000	1.00	0.00
ILE93	HD11	0.99	0.000	1.00	0.00
ILE93	H	1.00	0.000	1.00	0.00
MET94	H	0.99	0.000	1.00	0.00
MET94	HA	0.70	0.010	1.00	0.00

**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	0.00
ILE93	HB	1.00	0.000	1.00	0.00
ILE93	HG12	1.00	0.000	1.00	0.00
ILE93	HG13	1.00	0.000	1.00	0.00
ILE93	HG21	0.99	0.000	1.00	0.00
ILE93	HD11	1.00	0.000	1.00	0.00
ILE93	H	0.94	0.000	1.00	0.00

**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	0.000	1.00	0.00
THR92	HB	1.00	0.000	1.00	0.00
THR92	HG21	0.98	0.000	1.00	0.00
THR92	H	1.00	0.000	1.00	0.00
ILE93	HA	1.00	0.000	1.00	0.00
ILE93	HB	1.00	0.000	1.00	0.00
ILE93	HG12	1.00	0.000	1.00	0.00
ILE93	HG13	1.00	0.000	1.00	0.00
ILE93	HG21	1.00	0.000	1.00	0.00
ILE93	H	1.00	0.000	1.00	0.00
ILE93	HD11	0.94	0.000	1.00	0.00
MET94	H	1.00	0.000	1.00	0.00

**3.93.7 Detailed Probabilities of ILE93HA:**

Overall probability: 0.800

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR92	0.00	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	0.454	0.00	0.00
ILE93	HA	1.00	0.000	1.00	0.00
ILE93	HB	1.00	0.000	1.00	0.00
ILE93	HG12	1.00	0.000	1.00	0.00
ILE93	HG13	1.00	0.000	1.00	0.00
ILE93	HG21	1.00	0.000	1.00	0.00
ILE93	HD11	0.97	0.000	1.00	0.00
ILE93	H	1.00	0.000	1.00	0.00
MET94	HA	1.00	0.341	0.00	0.00
MET94	H	1.00	0.000	1.00	0.00

**3.93.8 Detailed Probabilities of ILE93HB:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE93	1.00	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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE93	HA	1.00	0.000	1.00	0.00
ILE93	HB	1.00	0.000	1.00	0.00
ILE93	HG12	1.00	0.000	1.00	0.00
ILE93	HG13	1.00	0.000	1.00	0.00
ILE93	HG21	1.00	0.000	1.00	0.00
ILE93	HD11	1.00	0.000	1.00	0.00
ILE93	H	1.00	0.000	1.00	0.00
MET94	H	1.00	0.000	1.00	0.00

## 3.93.9 Detailed Probabilities of ILE93HG12:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
ILE93	1.00	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	0.000	1.00	0.00
ILE93	HB	1.00	0.000	1.00	0.00
ILE93	HG12	1.00	0.000	1.00	0.00
ILE93	HG13	1.00	0.000	1.00	0.00
ILE93	HG21	1.00	0.000	1.00	0.00
ILE93	HD11	1.00	0.000	1.00	0.00
ILE93	H	1.00	0.000	1.00	0.00
MET94	H	0.97	0.000	1.00	0.00

## 3.93.10 Detailed Probabilities of ILE93HG13:

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	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	0.000	1.00	0.00
ILE93	HB	1.00	0.000	1.00	0.00
ILE93	HG12	1.00	0.000	1.00	0.00
ILE93	HG13	1.00	0.000	1.00	0.00
ILE93	HG21	1.00	0.000	1.00	0.00
ILE93	HD11	1.00	0.000	1.00	0.00
ILE93	H	1.00	0.000	1.00	0.00

**3.93.11 Detailed Probabilities of ILE93HG21:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE93	1.00	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	0.000	1.00	0.00
ILE93	HB	1.00	0.000	1.00	0.00
ILE93	HG12	1.00	0.000	1.00	0.00
ILE93	HG13	1.00	0.000	1.00	0.00
ILE93	HG21	1.00	0.000	1.00	0.00
ILE93	HD11	0.99	0.000	1.00	0.00
ILE93	H	1.00	0.000	1.00	0.00
MET94	H	0.99	0.000	1.00	0.00
MET94	HA	0.70	0.000	1.00	0.00

**3.93.12 Detailed Probabilities of ILE93HD11:**

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	0.00
ILE93	HB	1.00	0.000	1.00	0.00
ILE93	HG12	1.00	0.000	1.00	0.00
ILE93	HG13	1.00	0.000	1.00	0.00
ILE93	HG21	0.99	0.000	1.00	0.00
ILE93	HD11	1.00	0.000	1.00	0.00
ILE93	H	0.94	0.000	1.00	0.00

**3.93.13 Detailed Probabilities of ILE93H:**

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	0.000	1.00	0.00
THR92	HB	1.00	0.000	1.00	0.00
THR92	HG21	0.98	0.000	1.00	0.00
THR92	H	1.00	0.000	1.00	0.00
ILE93	HA	1.00	0.000	1.00	0.00
ILE93	HB	1.00	0.000	1.00	0.00
ILE93	HG12	1.00	0.000	1.00	0.00
ILE93	HG13	1.00	0.000	1.00	0.00
ILE93	HG21	1.00	0.000	1.00	0.00
ILE93	H	1.00	0.000	1.00	0.00
ILE93	HD11	0.94	0.000	1.00	0.00
MET94	H	1.00	0.000	1.00	0.00
MET94	HA	0.91	0.018	1.00	0.00

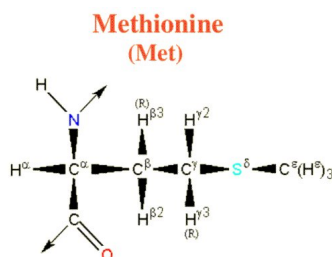


Figure 84: Image from the BMRB

Residue probability: 0.965  
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	0.833	1.000
CB 3.94.2	31.488	33.217	4.564	1.000	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	1.000	1.000
N 3.94.5	118.345	120.023	5.158	1.000	1.000
HA 3.94.6	4.279	4.409	0.504	0.818	1.000
HB2 3.94.7	2.121	2.016	0.340	1.000	1.000
HB3 3.94.8	2.032	1.978	0.359	1.000	1.000
HG2 3.94.9	2.524	2.410	0.360	1.000	1.000
HG3 3.94.10	2.666	2.378	0.386	1.000	1.000
HE 3.94.11	2.024	1.877	0.381	1.000	1.000
H 3.94.12	8.632	8.269	0.585	0.931	1.000

**3.94.1 Detailed Probabilities of MET94CA:**

Overall probability: 0.833  
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	0.341	0.00	0.00
ILE93	HG21	0.73	0.000	1.00	0.00
ILE93	H	0.91	0.018	1.00	0.00
MET94	HA	1.00	0.000	1.00	0.00
MET94	HB2	1.00	0.000	1.00	0.00
MET94	HB3	1.00	0.000	1.00	0.00
MET94	HG2	1.00	0.000	1.00	0.00
MET94	HG3	1.00	0.000	1.00	0.00
MET94	H	1.00	0.000	1.00	0.00
MET94	HE1	0.69	0.000	1.00	0.00
ASP95	HA	1.00	0.133	0.00	0.00
ASP95	H	1.00	0.000	1.00	0.00

**3.94.2 Detailed Probabilities of MET94CB:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
MET94	1.00	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**

## 3.94 MET(94)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET94	HA	1.00	0.000	1.00	0.00
MET94	HB2	1.00	0.000	1.00	0.00
MET94	HB3	1.00	0.000	1.00	0.00
MET94	HG2	1.00	0.000	1.00	0.00
MET94	HG3	1.00	0.000	1.00	0.00
MET94	HE1	0.96	0.000	1.00	0.00
MET94	H	1.00	0.000	1.00	0.00
ASP95	H	1.00	0.000	1.00	0.00

## 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
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	0.000	1.00	0.00
MET94	HB2	1.00	0.000	1.00	0.00
MET94	HB3	1.00	0.000	1.00	0.00
MET94	HG2	1.00	0.000	1.00	0.00
MET94	HG3	1.00	0.000	1.00	0.00
MET94	HE1	1.00	0.000	1.00	0.00
MET94	H	1.00	0.000	1.00	0.00
ASP95	H	0.97	0.000	1.00	0.00

## 3.94.4 Detailed Probabilities of MET94CE:

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
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	0.000	1.00	0.00
MET94	HB3	0.97	0.000	1.00	0.00
MET94	HG2	1.00	0.000	1.00	0.00
MET94	HG3	1.00	0.000	1.00	0.00
MET94	HE1	1.00	0.000	1.00	0.00
MET94	HA	0.67	0.000	1.00	0.00

**3.94.5 Detailed Probabilities of MET94N:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE93	1.00	1.00
MET94	1.00	1.00
ASP95	1.00	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**

## 3.94 MET(94)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE93	HA	1.00	0.000	1.00	0.00
ILE93	HB	1.00	0.000	1.00	0.00
ILE93	HG12	0.97	0.000	1.00	0.00
ILE93	HG21	0.98	0.000	1.00	0.00
ILE93	H	1.00	0.000	1.00	0.00
ILE93	HG13	0.93	0.000	1.00	0.00
MET94	HA	1.00	0.000	1.00	0.00
MET94	HB2	1.00	0.000	1.00	0.00
MET94	HB3	1.00	0.000	1.00	0.00
MET94	HG2	1.00	0.000	1.00	0.00
MET94	HG3	1.00	0.000	1.00	0.00
MET94	H	1.00	0.000	1.00	0.00
ASP95	H	1.00	0.000	1.00	0.00

## 3.94.6 Detailed Probabilities of MET94HA:

Overall probability: 0.818

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
ILE93	0.50	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	0.756	0.00	0.00
ILE93	HG21	0.73	0.010	1.00	0.00
MET94	HA	1.00	0.000	1.00	0.00
MET94	HB2	1.00	0.000	1.00	0.00
MET94	HB3	1.00	0.000	1.00	0.00
MET94	HG2	1.00	0.000	1.00	0.00
MET94	HG3	1.00	0.000	1.00	0.00
MET94	H	1.00	0.000	1.00	0.00
MET94	HE1	0.69	0.000	1.00	0.00
ASP95	HA	1.00	0.133	0.00	0.00
ASP95	H	1.00	0.000	1.00	0.00

**3.94.7 Detailed Probabilities of MET94HB2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
MET94	1.00	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	0.000	1.00	0.00
MET94	HB2	1.00	0.000	1.00	0.00
MET94	HB3	1.00	0.000	1.00	0.00
MET94	HG2	1.00	0.000	1.00	0.00
MET94	HG3	1.00	0.000	1.00	0.00
MET94	HE1	0.96	0.000	1.00	0.00
MET94	H	1.00	0.000	1.00	0.00
ASP95	H	1.00	0.000	1.00	0.00

**3.94.8 Detailed Probabilities of MET94HB3:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
MET94	1.00	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	0.000	1.00	0.00
MET94	HB2	1.00	0.000	1.00	0.00
MET94	HB3	1.00	0.000	1.00	0.00
MET94	HG2	1.00	0.000	1.00	0.00
MET94	HG3	1.00	0.000	1.00	0.00
MET94	HE1	0.97	0.000	1.00	0.00
MET94	H	1.00	0.000	1.00	0.00
ASP95	H	1.00	0.000	1.00	0.00

**3.94.9 Detailed Probabilities of MET94HG2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
MET94	1.00	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	0.000	1.00	0.00
MET94	HB2	1.00	0.000	1.00	0.00
MET94	HB3	1.00	0.000	1.00	0.00
MET94	HG2	1.00	0.000	1.00	0.00
MET94	HG3	1.00	0.000	1.00	0.00
MET94	HE1	1.00	0.000	1.00	0.00
MET94	H	1.00	0.000	1.00	0.00
ASP95	H	0.97	0.000	1.00	0.00

**3.94.10 Detailed Probabilities of MET94HG3:**

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	0.000	1.00	0.00
MET94	HB2	1.00	0.000	1.00	0.00
MET94	HB3	1.00	0.000	1.00	0.00
MET94	HG2	1.00	0.000	1.00	0.00
MET94	HG3	1.00	0.000	1.00	0.00
MET94	HE1	1.00	0.000	1.00	0.00
MET94	H	1.00	0.000	1.00	0.00

**3.94.11 Detailed Probabilities of MET94HE1:**

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
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	0.000	1.00	0.00
MET94	HB3	0.97	0.000	1.00	0.00
MET94	HG2	1.00	0.000	1.00	0.00
MET94	HG3	1.00	0.000	1.00	0.00
MET94	HE1	1.00	0.000	1.00	0.00
MET94	HA	0.67	0.000	1.00	0.00

**3.94.12 Detailed Probabilities of MET94H:**

Overall probability: 0.931

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ILE93	0.84	1.00
MET94	1.00	1.00
ASP95	1.00	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	0.000	1.00	0.00
ILE93	HB	1.00	0.000	1.00	0.00
ILE93	HG12	0.97	0.379	0.03	0.00
ILE93	HG21	0.98	0.000	1.00	0.00
ILE93	H	1.00	0.000	1.00	0.00
ILE93	HG13	0.93	0.000	1.00	0.00
MET94	HA	1.00	0.000	1.00	0.00
MET94	HB2	1.00	0.000	1.00	0.00
MET94	HB3	1.00	0.000	1.00	0.00
MET94	HG2	1.00	0.000	1.00	0.00
MET94	HG3	1.00	0.000	1.00	0.00
MET94	H	1.00	0.000	1.00	0.00
ASP95	H	1.00	0.000	1.00	0.00
ASP95	HA	0.85	0.008	1.00	0.00

**3.95 ASP(95)**

Figure 85: Image from the BMRB

Residue probability: 0.923

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	0.750	0.875
CB 3.95.2	40.075	40.949	3.070	1.000	0.833
N 3.95.3	120.052	120.550	5.690	1.000	1.000
HD2	NA	—	—	0.000	0.000
HA 3.95.4	4.412	4.587	0.329	0.714	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	1.000	1.000

**3.95.1 Detailed Probabilities of ASP95CA:**

Overall probability: 0.750

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
MET94	0.50	1.00
ASP95	1.00	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	0.133	0.00	0.00
MET94	H	0.85	0.008	1.00	0.00
ASP95	HA	1.00	0.000	1.00	0.00
ASP95	HB2	1.00	0.000	1.00	0.00
ASP95	HB3	1.00	0.000	1.00	0.00
ASP95	H	1.00	0.000	1.00	0.00
PHE96	HA	1.00	0.352	0.00	0.00
PHE96	H	1.00	0.000	1.00	0.00

**3.95.2 Detailed Probabilities of ASP95CB:**

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	0.000	1.00	0.00
ASP95	HB2	1.00	0.000	1.00	0.00
ASP95	HB3	1.00	0.000	1.00	0.00
ASP95	H	1.00	0.000	1.00	0.00
PHE96	H	1.00	0.000	1.00	0.00

**3.95.3 Detailed Probabilities of ASP95N:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
MET94	1.00	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	0.000	1.00	0.00
MET94	HB2	1.00	0.000	1.00	0.00
MET94	HB3	1.00	0.000	1.00	0.00
MET94	HG2	0.97	0.000	1.00	0.00
MET94	H	1.00	0.000	1.00	0.00
MET94	HG3	0.95	0.000	1.00	0.00
ASP95	HA	1.00	0.000	1.00	0.00
ASP95	HB2	1.00	0.000	1.00	0.00
ASP95	HB3	1.00	0.000	1.00	0.00
ASP95	H	1.00	0.000	1.00	0.00
PHE96	H	1.00	0.000	1.00	0.00
PHE96	HA	0.88	0.021	1.00	0.00

**3.95.4 Detailed Probabilities of ASP95HA:**

Overall probability: 0.714

Overall confidence: 0.875

**Inter- and intra-residue probability**

Residue	Probability	Confidence
MET94	0.00	1.00
ASP95	1.00	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	0.133	0.00	0.00
ASP95	HA	1.00	0.000	1.00	0.00
ASP95	HB2	1.00	0.000	1.00	0.00
ASP95	HB3	1.00	0.000	1.00	0.00
ASP95	H	1.00	0.000	1.00	0.00
PHE96	HA	1.00	0.352	0.00	0.00
PHE96	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ASP95	HB2	1.00	0.000	1.00	0.00
ASP95	HB3	1.00	0.000	1.00	0.00
ASP95	H	1.00	0.000	1.00	0.00
PHE96	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ASP95	HB2	1.00	0.000	1.00	0.00
ASP95	HB3	1.00	0.000	1.00	0.00
ASP95	H	1.00	0.000	1.00	0.00
PHE96	H	1.00	0.000	1.00	0.00
PHE96	HA	0.83	0.016	1.00	0.00

**3.95.7 Detailed Probabilities of ASP95H:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
MET94	1.00	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**

## 3.95 ASP(95)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET94	HA	1.00	0.000	1.00	0.00
MET94	HB2	1.00	0.000	1.00	0.00
MET94	HB3	1.00	0.000	1.00	0.00
MET94	HG2	0.97	0.000	1.00	0.00
MET94	H	1.00	0.000	1.00	0.00
MET94	HG3	0.95	0.000	1.00	0.00
ASP95	HA	1.00	0.000	1.00	0.00
ASP95	HB2	1.00	0.000	1.00	0.00
ASP95	HB3	1.00	0.000	1.00	0.00
ASP95	H	1.00	0.000	1.00	0.00
PHE96	H	1.00	0.000	1.00	0.00

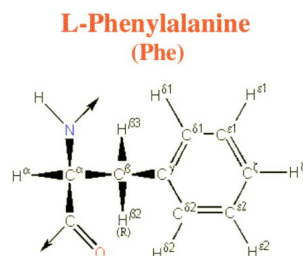


Figure 86: Image from the BMRB

Residue probability: 0.935  
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	0.850	1.000
CB 3.96.2	39.421	40.078	3.616	1.000	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	1.000	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	0.850	1.000
HB2 3.96.10	3.252	2.980	0.399	0.875	1.000
HB3 3.96.11	2.945	2.916	0.434	1.000	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	1.000	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	0.820	1.000

### 3.96.1 Detailed Probabilities of PHE96CA:

Overall probability: 0.850  
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP95	0.50	1.00
PHE96	1.00	1.00
PHE97	0.75	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	0.352	0.00	0.00
ASP95	HB3	0.83	0.016	1.00	0.00
PHE96	HA	1.00	0.000	1.00	0.00
PHE96	HB2	1.00	0.000	1.00	0.00
PHE96	HB3	1.00	0.000	1.00	0.00
PHE96	HD1	1.00	0.003	1.00	0.00
PHE96	HD2	1.00	0.003	1.00	0.00
PHE96	H	1.00	0.000	1.00	0.00
PHE97	HA	1.00	0.035	0.50	0.00
PHE97	H	1.00	0.000	1.00	0.00

**3.96.2 Detailed Probabilities of PHE96CB:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE96	1.00	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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE96	HA	1.00	0.000	1.00	0.00
PHE96	HB2	1.00	0.000	1.00	0.00
PHE96	HB3	1.00	0.000	1.00	0.00
PHE96	HD1	1.00	0.003	1.00	0.00
PHE96	HD2	1.00	0.003	1.00	0.00
PHE96	HE2	1.00	0.012	1.00	0.00
PHE96	H	1.00	0.000	1.00	0.00
PHE96	HE1	0.90	0.012	1.00	0.00
PHE97	H	1.00	0.000	1.00	0.00

## 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	0.000	1.00	0.00
PHE96	HB2	1.00	0.000	1.00	0.00
PHE96	HB3	1.00	0.000	1.00	0.00
PHE96	HD1	1.00	0.003	1.00	0.00
PHE96	HD2	1.00	0.003	1.00	0.00
PHE96	HE1	1.00	0.004	1.00	0.00
PHE96	HE2	1.00	0.004	1.00	0.00
PHE96	HZ	1.00	0.002	1.00	0.00
PHE96	H	1.00	1.265	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	0.000	1.00	0.00
PHE96	HB2	1.00	0.000	1.00	0.00
PHE96	HB3	1.00	0.000	1.00	0.00
PHE96	HD1	1.00	0.003	1.00	0.00
PHE96	HD2	1.00	0.003	1.00	0.00
PHE96	HE1	1.00	0.004	1.00	0.00
PHE96	HE2	1.00	0.004	1.00	0.00
PHE96	HZ	1.00	0.002	1.00	0.00
PHE96	H	0.99	1.265	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	0.003	1.00	0.00
PHE96	HD2	1.00	0.003	1.00	0.00
PHE96	HE1	1.00	0.004	1.00	0.00
PHE96	HE2	1.00	0.004	1.00	0.00
PHE96	HZ	1.00	0.002	1.00	0.00
PHE96	HB3	0.89	0.011	1.00	0.00

**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	0.296	0.00	0.00
PHE96	HB3	1.00	0.011	1.00	0.00
PHE96	HD1	1.00	0.003	1.00	0.00
PHE96	HD2	1.00	0.003	1.00	0.00
PHE96	HE1	1.00	0.004	1.00	0.00
PHE96	HE2	1.00	0.004	1.00	0.00
PHE96	HZ	1.00	0.002	1.00	0.00

**3.96.7 Detailed Probabilities of PHE96CZ:**

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	0.003	1.00	0.00
PHE96	HD2	1.00	0.003	1.00	0.00
PHE96	HE1	1.00	0.004	1.00	0.00
PHE96	HE2	1.00	0.004	1.00	0.00
PHE96	HZ	1.00	0.002	1.00	0.00

**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	0.000	1.00	0.00
ASP95	HB2	1.00	0.000	1.00	0.00
ASP95	HB3	1.00	0.000	1.00	0.00
ASP95	H	1.00	0.000	1.00	0.00
PHE96	HA	1.00	0.000	1.00	0.00
PHE96	HB2	1.00	0.000	1.00	0.00
PHE96	HB3	1.00	0.000	1.00	0.00
PHE96	HD1	1.00	0.003	1.00	0.00
PHE96	HD2	0.99	0.003	1.00	0.00
PHE96	H	1.00	0.000	1.00	0.00
PHE97	H	1.00	0.000	1.00	0.00

**3.96.9 Detailed Probabilities of PHE96HA:**

Overall probability: 0.850

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASP95	0.50	1.00
PHE96	1.00	1.00
PHE97	0.75	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	0.352	0.00	0.00
ASP95	H	0.88	0.021	1.00	0.00
PHE96	HA	1.00	0.000	1.00	0.00
PHE96	HB2	1.00	0.000	1.00	0.00
PHE96	HB3	1.00	0.000	1.00	0.00
PHE96	HD1	1.00	0.000	1.00	0.00
PHE96	HD2	1.00	0.000	1.00	0.00
PHE96	H	1.00	0.000	1.00	0.00
PHE97	HA	1.00	0.035	0.50	0.00
PHE97	H	1.00	0.000	1.00	0.00

**3.96.10 Detailed Probabilities of PHE96HB2:**

Overall probability: 0.875

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE96	0.86	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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE96	HA	1.00	0.000	1.00	0.00
PHE96	HB2	1.00	0.000	1.00	0.00
PHE96	HB3	1.00	0.000	1.00	0.00
PHE96	HD1	1.00	0.000	1.00	0.00
PHE96	HD2	1.00	0.000	1.00	0.00
PHE96	HE2	1.00	0.296	0.00	0.00
PHE96	H	1.00	0.000	1.00	0.00
PHE97	H	1.00	0.000	1.00	0.00

## 3.96.11 Detailed Probabilities of PHE96HB3:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
PHE96	1.00	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	0.000	1.00	0.00
PHE96	HB2	1.00	0.000	1.00	0.00
PHE96	HB3	1.00	0.000	1.00	0.00
PHE96	HD1	1.00	0.000	1.00	0.00
PHE96	HD2	1.00	0.000	1.00	0.00
PHE96	HE2	1.00	0.011	1.00	0.00
PHE96	H	1.00	0.000	1.00	0.00
PHE96	HE1	0.89	0.011	1.00	0.00
PHE97	H	1.00	0.000	1.00	0.00

## 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	0.003	1.00	0.00
PHE96	HB2	1.00	0.003	1.00	0.00
PHE96	HB3	1.00	0.003	1.00	0.00
PHE96	HD1	1.00	0.003	1.00	0.00
PHE96	HD2	1.00	0.003	1.00	0.00
PHE96	HE1	1.00	0.003	1.00	0.00
PHE96	HE2	1.00	0.003	1.00	0.00
PHE96	HZ	1.00	0.003	1.00	0.00
PHE96	H	1.00	0.003	1.00	0.00

**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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE96	HA	1.00	0.003	1.00	0.00
PHE96	HB2	1.00	0.003	1.00	0.00
PHE96	HB3	1.00	0.003	1.00	0.00
PHE96	HD1	1.00	0.003	1.00	0.00
PHE96	HD2	1.00	0.003	1.00	0.00
PHE96	HE1	1.00	0.003	1.00	0.00
PHE96	HE2	1.00	0.003	1.00	0.00
PHE96	HZ	1.00	0.003	1.00	0.00
PHE96	H	0.99	0.003	1.00	0.00

## 3.96.14 Detailed Probabilities of PHE96HE1:

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	0.004	1.00	0.00
PHE96	HD2	1.00	0.004	1.00	0.00
PHE96	HE1	1.00	0.004	1.00	0.00
PHE96	HE2	1.00	0.004	1.00	0.00
PHE96	HZ	1.00	0.004	1.00	0.00
PHE96	HB2	0.90	0.012	1.00	0.00

## 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	0.012	1.00	0.00
PHE96	HB3	1.00	0.186	0.00	0.00
PHE96	HD1	1.00	0.004	1.00	0.00
PHE96	HD2	1.00	0.004	1.00	0.00
PHE96	HE1	1.00	0.004	1.00	0.00
PHE96	HE2	1.00	0.004	1.00	0.00
PHE96	HZ	1.00	0.004	1.00	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	0.002	1.00	0.00
PHE96	HD2	1.00	0.002	1.00	0.00
PHE96	HE1	1.00	0.002	1.00	0.00
PHE96	HE2	1.00	0.002	1.00	0.00
PHE96	HZ	1.00	0.002	1.00	0.00

**3.96.17 Detailed Probabilities of PHE96H:**

Overall probability: 0.820

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASP95	1.00	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	0.000	1.00	0.00
ASP95	HB2	1.00	0.000	1.00	0.00
ASP95	HB3	1.00	0.000	1.00	0.00
ASP95	H	1.00	0.000	1.00	0.00
PHE96	HA	1.00	0.000	1.00	0.00
PHE96	HB2	1.00	0.000	1.00	0.00
PHE96	HB3	1.00	0.000	1.00	0.00
PHE96	HD1	1.00	1.265	0.00	0.00
PHE96	HD2	0.99	1.265	0.01	0.00
PHE96	H	1.00	0.000	1.00	0.00
PHE97	H	1.00	0.000	1.00	0.00

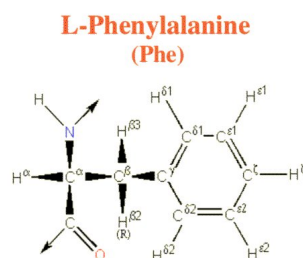


Figure 87: Image from the BMRB

Residue probability: 0.926  
 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	0.850	1.000
CB 3.97.2	37.867	40.078	3.616	0.875	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	1.000	1.000
CE2 3.97.6	130.815	130.633	2.839	0.715	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	1.000	1.000
HA 3.97.9	4.025	4.625	1.237	0.837	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	1.000	1.000
HD2 3.97.13	7.579	7.022	0.417	1.000	1.000
HE1 3.97.14	7.217	7.046	0.417	1.000	1.000
HE2 3.97.15	7.217	7.043	0.400	0.715	1.000
HZ 3.97.16	7.002	6.984	1.598	1.000	1.000
H 3.97.17	8.624	8.375	0.710	1.000	1.000

**3.97.1 Detailed Probabilities of PHE97CA:**

Overall probability: 0.850  
 Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE96	0.50	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	0.035	0.50	0.00
PHE97	HA	1.00	0.000	1.00	0.00
PHE97	HB2	1.00	0.000	1.00	0.00
PHE97	HB3	1.00	0.000	1.00	0.00
PHE97	HD1	1.00	0.000	1.00	0.00
PHE97	HD2	1.00	0.000	1.00	0.00
PHE97	H	1.00	0.000	1.00	0.00
PHE97	HE1	0.74	0.000	1.00	0.00
ALA98	HA	1.00	0.222	0.00	0.00
ALA98	H	1.00	0.000	1.00	0.00

**3.97.2 Detailed Probabilities of PHE97CB:**

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)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE97	HA	1.00	0.000	1.00	0.00
PHE97	HB2	1.00	0.000	1.00	0.00
PHE97	HB3	1.00	0.000	1.00	0.00
PHE97	HD1	1.00	0.000	1.00	0.00
PHE97	HD2	1.00	0.000	1.00	0.00
PHE97	HE2	1.00	0.208	0.00	0.00
PHE97	H	1.00	0.000	1.00	0.00
ALA98	H	1.00	0.000	1.00	0.00

## 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	0.000	1.00	0.00
PHE97	HB2	1.00	0.000	1.00	0.00
PHE97	HB3	1.00	0.000	1.00	0.00
PHE97	HD1	1.00	0.000	1.00	0.00
PHE97	HD2	1.00	0.000	1.00	0.00
PHE97	HE1	1.00	0.000	1.00	0.00
PHE97	HE2	1.00	0.000	1.00	0.00
PHE97	HZ	1.00	0.000	1.00	0.00
PHE97	H	1.00	0.000	1.00	0.00

## 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	0.000	1.00	0.00
PHE97	HB2	1.00	0.000	1.00	0.00
PHE97	HB3	1.00	0.000	1.00	0.00
PHE97	HD1	1.00	0.000	1.00	0.00
PHE97	HD2	1.00	0.000	1.00	0.00
PHE97	HE1	1.00	0.000	1.00	0.00
PHE97	HE2	1.00	0.000	1.00	0.00
PHE97	HZ	1.00	0.000	1.00	0.00
PHE97	H	0.99	0.000	1.00	0.00

**3.97.5 Detailed Probabilities of PHE97CE1:**

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
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	0.000	1.00	0.00
PHE97	HD2	1.00	0.000	1.00	0.00
PHE97	HE1	1.00	0.000	1.00	0.00
PHE97	HE2	1.00	0.000	1.00	0.00
PHE97	HZ	1.00	0.000	1.00	0.00
PHE97	HA	0.74	0.000	1.00	0.00

**3.97.6 Detailed Probabilities of PHE97CE2:**

Overall probability: 0.715

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE97	0.71	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	0.993	0.00	0.00
PHE97	HB3	1.00	0.843	0.00	0.00
PHE97	HD1	1.00	0.000	1.00	0.00
PHE97	HD2	1.00	0.000	1.00	0.00
PHE97	HE1	1.00	0.000	1.00	0.00
PHE97	HE2	1.00	0.000	1.00	0.00
PHE97	HZ	1.00	0.000	1.00	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	0.000	1.00	0.00
PHE97	HD2	1.00	0.000	1.00	0.00
PHE97	HE1	1.00	0.000	1.00	0.00
PHE97	HE2	1.00	0.000	1.00	0.00
PHE97	HZ	1.00	0.000	1.00	0.00

**3.97.8 Detailed Probabilities of PHE97N:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE96	1.00	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	0.000	1.00	0.00
PHE96	HB2	1.00	0.000	1.00	0.00
PHE96	HB3	1.00	0.000	1.00	0.00
PHE96	H	1.00	0.000	1.00	0.00
PHE96	HD1	0.79	0.003	1.00	0.00
PHE96	HD2	0.70	0.003	1.00	0.00
PHE97	HA	1.00	0.000	1.00	0.00
PHE97	HB2	1.00	0.000	1.00	0.00
PHE97	HB3	1.00	0.000	1.00	0.00
PHE97	HD1	1.00	0.000	1.00	0.00
PHE97	HD2	0.99	0.000	1.00	0.00
PHE97	H	1.00	0.000	1.00	0.00
ALA98	H	1.00	0.000	1.00	0.00

**3.97.9 Detailed Probabilities of PHE97HA:**

Overall probability: 0.837

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE96	0.72	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	0.035	0.50	0.00
PHE96	HB2	0.59	0.035	0.59	0.00
PHE96	HB3	0.88	0.035	0.88	0.00
PHE96	H	0.90	0.035	0.90	0.00
PHE97	HA	1.00	0.000	1.00	0.00
PHE97	HB2	1.00	0.000	1.00	0.00
PHE97	HB3	1.00	0.000	1.00	0.00
PHE97	HD1	1.00	0.000	1.00	0.00
PHE97	HD2	1.00	0.000	1.00	0.00
PHE97	H	1.00	0.000	1.00	0.00
PHE97	HE1	0.74	0.000	1.00	0.00
ALA98	HA	1.00	0.222	0.00	0.00
ALA98	H	1.00	0.000	1.00	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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE97	HA	1.00	0.000	1.00	0.00
PHE97	HB2	1.00	0.000	1.00	0.00
PHE97	HB3	1.00	0.000	1.00	0.00
PHE97	HD1	1.00	0.000	1.00	0.00
PHE97	HD2	1.00	0.000	1.00	0.00
PHE97	HE2	1.00	0.993	0.00	0.00
PHE97	H	1.00	0.000	1.00	0.00
ALA98	H	1.00	0.000	1.00	0.00

**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	0.00
PHE97	HB2	1.00	0.000	1.00	0.00
PHE97	HB3	1.00	0.000	1.00	0.00
PHE97	HD1	1.00	0.000	1.00	0.00
PHE97	HD2	1.00	0.000	1.00	0.00
PHE97	HE2	1.00	0.843	0.00	0.00
PHE97	H	1.00	0.000	1.00	0.00
ALA98	H	1.00	0.000	1.00	0.00

**3.97.12 Detailed Probabilities of PHE97HD1:**

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	0.000	1.00	0.00
PHE97	HB2	1.00	0.000	1.00	0.00
PHE97	HB3	1.00	0.000	1.00	0.00
PHE97	HD1	1.00	0.000	1.00	0.00
PHE97	HD2	1.00	0.000	1.00	0.00
PHE97	HE1	1.00	0.000	1.00	0.00
PHE97	HE2	1.00	0.000	1.00	0.00
PHE97	HZ	1.00	0.000	1.00	0.00
PHE97	H	1.00	0.000	1.00	0.00

**3.97.13 Detailed Probabilities of PHE97HD2:**

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**

## 3.97 PHE(97)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE97	HA	1.00	0.000	1.00	0.00
PHE97	HB2	1.00	0.000	1.00	0.00
PHE97	HB3	1.00	0.000	1.00	0.00
PHE97	HD1	1.00	0.000	1.00	0.00
PHE97	HD2	1.00	0.000	1.00	0.00
PHE97	HE1	1.00	0.000	1.00	0.00
PHE97	HE2	1.00	0.000	1.00	0.00
PHE97	HZ	1.00	0.000	1.00	0.00
PHE97	H	0.99	0.000	1.00	0.00

## 3.97.14 Detailed Probabilities of PHE97HE1:

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
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	0.000	1.00	0.00
PHE97	HD2	1.00	0.000	1.00	0.00
PHE97	HE1	1.00	0.000	1.00	0.00
PHE97	HE2	1.00	0.000	1.00	0.00
PHE97	HZ	1.00	0.000	1.00	0.00
PHE97	HA	0.74	0.000	1.00	0.00

## 3.97.15 Detailed Probabilities of PHE97HE2:

Overall probability: 0.715

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
PHE97	0.71	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	0.208	0.00	0.00
PHE97	HB3	1.00	0.208	0.00	0.00
PHE97	HD1	1.00	0.000	1.00	0.00
PHE97	HD2	1.00	0.000	1.00	0.00
PHE97	HE1	1.00	0.000	1.00	0.00
PHE97	HE2	1.00	0.000	1.00	0.00
PHE97	HZ	1.00	0.000	1.00	0.00

**3.97.16 Detailed Probabilities of PHE97HZ:**

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	0.000	1.00	0.00
PHE97	HD2	1.00	0.000	1.00	0.00
PHE97	HE1	1.00	0.000	1.00	0.00
PHE97	HE2	1.00	0.000	1.00	0.00
PHE97	HZ	1.00	0.000	1.00	0.00

**3.97.17 Detailed Probabilities of PHE97H:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE96	1.00	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	0.000	1.00	0.00
PHE96	HB2	1.00	0.000	1.00	0.00
PHE96	HB3	1.00	0.000	1.00	0.00
PHE96	H	1.00	0.000	1.00	0.00
PHE97	HA	1.00	0.000	1.00	0.00
PHE97	HB2	1.00	0.000	1.00	0.00
PHE97	HB3	1.00	0.000	1.00	0.00
PHE97	HD1	1.00	0.000	1.00	0.00
PHE97	HD2	0.99	0.000	1.00	0.00
PHE97	H	1.00	0.000	1.00	0.00
ALA98	H	1.00	0.000	1.00	0.00

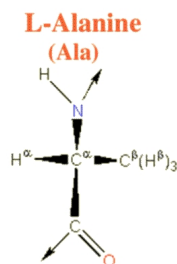
**3.98 ALA(98)**

Figure 88: 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
CA 3.98.1	53.463	53.289	3.425	0.667	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	1.000	1.000
HA 3.98.4	4.247	4.254	0.459	0.716	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	1.000	1.000

**3.98.1 Detailed Probabilities of ALA98CA:**

Overall probability: 0.667

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PHE97	0.00	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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE97	HA	1.00	0.222	0.00	0.00
ALA98	HA	1.00	0.000	1.00	0.00
ALA98	HB1	1.00	0.000	1.00	0.00
ALA98	H	1.00	0.000	1.00	0.00
SER99	HA	1.00	0.102	0.00	0.00
SER99	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
ALA98	HB1	1.00	0.000	1.00	0.00
ALA98	H	1.00	0.000	1.00	0.00
SER99	H	1.00	0.000	1.00	0.00

**3.98.3 Detailed Probabilities of ALA98N:**

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
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	0.000	1.00	0.00
PHE97	HB2	1.00	0.000	1.00	0.00
PHE97	HB3	1.00	0.000	1.00	0.00
PHE97	H	1.00	0.000	1.00	0.00
ALA98	HA	1.00	0.000	1.00	0.00
ALA98	HB1	1.00	0.000	1.00	0.00
ALA98	H	1.00	0.000	1.00	0.00
SER99	H	1.00	0.000	1.00	0.00

## 3.98.4 Detailed Probabilities of ALA98HA:

Overall probability: 0.716

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
PHE97	0.61	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	0.222	0.00	0.00
PHE97	HB2	0.61	0.032	0.80	0.00
PHE97	HB3	0.78	0.032	0.80	0.00
PHE97	H	0.84	0.032	0.84	0.00
ALA98	HA	1.00	0.000	1.00	0.00
ALA98	HB1	1.00	0.000	1.00	0.00
ALA98	H	1.00	0.000	1.00	0.00
SER99	HA	1.00	0.098	0.00	0.00
SER99	H	1.00	0.000	1.00	0.00

## 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	0.00
ALA98	HB1	1.00	0.000	1.00	0.00
ALA98	H	1.00	0.000	1.00	0.00
SER99	H	1.00	0.000	1.00	0.00
SER99	HA	0.70	0.007	1.00	0.00

**3.98.6 Detailed Probabilities of ALA98H:**

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
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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE97	HA	1.00	0.000	1.00	0.00
PHE97	HB2	1.00	0.000	1.00	0.00
PHE97	HB3	1.00	0.000	1.00	0.00
PHE97	H	1.00	0.000	1.00	0.00
ALA98	HA	1.00	0.000	1.00	0.00
ALA98	HB1	1.00	0.000	1.00	0.00
ALA98	H	1.00	0.000	1.00	0.00
SER99	H	1.00	0.000	1.00	0.00

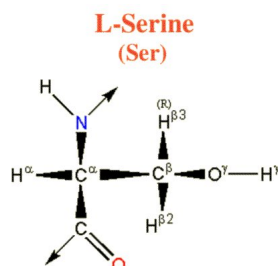
**3.99 SER(99)**

Figure 89: Image from the BMRB

Residue probability: 0.907

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	0.833	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	0.625	0.889
HB2 3.99.5	3.975	3.856	0.325	1.000	0.833
HB3 3.99.6	3.808	3.825	0.343	1.000	0.833
H 3.99.7	7.536	8.292	0.600	1.000	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	0.098	0.00	0.00
ALA98	HB1	0.66	0.007	1.00	0.00
SER99	HA	1.00	0.000	1.00	0.00
SER99	HB2	1.00	0.000	1.00	0.00
SER99	HB3	1.00	0.000	1.00	0.00
SER99	H	1.00	0.000	1.00	0.00
GLY100	HA2	1.00	0.012	1.00	0.00
GLY100	HA3	1.00	0.022	1.00	0.00
GLY100	H	1.00	0.000	1.00	0.00

**3.99.2 Detailed Probabilities of SER99CB:**

Overall probability: 0.833

Overall confidence: 0.833

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER99	1.00	0.80
GLY100	0.50	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	0.000	1.00	0.00
SER99	HB2	1.00	0.000	1.00	0.00
SER99	HB3	1.00	0.000	1.00	0.00
SER99	H	1.00	0.000	1.00	0.00
GLY100	H	1.00	0.099	0.00	0.00
GLY100	HA3	0.53	0.022	1.00	0.00

**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	0.000	1.00	0.00
ALA98	HB1	1.00	0.000	1.00	0.00
ALA98	H	1.00	0.000	1.00	0.00
SER99	HA	1.00	0.000	1.00	0.00
SER99	HB2	1.00	0.000	1.00	0.00
SER99	HB3	1.00	0.000	1.00	0.00
SER99	H	1.00	0.000	1.00	0.00
GLY100	H	1.00	0.000	1.00	0.00
GLY100	HA2	0.68	0.015	1.00	0.00
GLY100	HA3	0.71	0.022	1.00	0.00

**3.99.4 Detailed Probabilities of SER99HA:**

Overall probability: 0.625

Overall confidence: 0.889

**Inter- and intra-residue probability**

Residue	Probability	Confidence
ALA98	0.00	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	0.102	0.00	0.00
SER99	HA	1.00	0.000	1.00	0.00
SER99	HB2	1.00	0.000	1.00	0.00
SER99	HB3	1.00	0.000	1.00	0.00
SER99	H	1.00	0.000	1.00	0.00
GLY100	HA2	1.00	0.148	0.00	0.00
GLY100	HA3	1.00	0.148	0.00	0.00
GLY100	H	1.00	0.000	1.00	0.00

## 3.99.5 Detailed Probabilities of SER99HB2:

Overall probability: 1.000

Overall confidence: 0.833

## Inter- and intra-residue probability

Residue	Probability	Confidence
SER99	1.00	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	0.000	1.00	0.00
SER99	HB2	1.00	0.000	1.00	0.00
SER99	HB3	1.00	0.000	1.00	0.00
SER99	H	1.00	0.000	1.00	0.00
GLY100	H	1.00	0.000	1.00	0.00
GLY100	HA2	0.56	0.022	1.00	0.00
GLY100	HA3	0.53	0.022	1.00	0.00

## 3.99.6 Detailed Probabilities of SER99HB3:

Overall probability: 1.000

Overall confidence: 0.833

## Inter- and intra-residue probability

Residue	Probability	Confidence
SER99	1.00	0.80
GLY100	1.00	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	0.00
SER99	HB2	1.00	0.000	1.00	0.00
SER99	HB3	1.00	0.000	1.00	0.00
SER99	H	1.00	0.000	1.00	0.00
GLY100	H	1.00	0.000	1.00	0.00

**3.99.7 Detailed Probabilities of SER99H:**

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	0.000	1.00	0.00
ALA98	HB1	1.00	0.000	1.00	0.00
ALA98	H	1.00	0.000	1.00	0.00
SER99	HA	1.00	0.000	1.00	0.00
SER99	HB2	1.00	0.000	1.00	0.00
SER99	HB3	1.00	0.000	1.00	0.00
SER99	H	1.00	0.000	1.00	0.00
GLY100	H	1.00	0.000	1.00	0.00

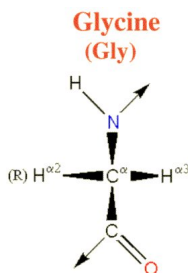


Figure 90: Image from the BMRB

Residue probability: 0.851  
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	0.750	1.000
N 3.100.2	109.375	109.752	5.331	1.000	0.889
HA2 3.100.3	3.702	3.967	0.380	0.857	1.000
HA3 3.100.4	3.997	3.897	0.390	0.900	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: 0.750  
Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER99	0.50	1.00
GLY100	1.00	1.00
LEU101	0.67	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	0.148	0.00	0.00
SER99	HB2	0.53	0.022	1.00	0.00
GLY100	HA2	1.00	0.000	1.00	0.00
GLY100	HA3	1.00	0.000	1.00	0.00
GLY100	H	1.00	0.000	1.00	0.00
LEU101	HA	1.00	0.364	0.00	0.00
LEU101	H	1.00	0.000	1.00	0.00
LEU101	HG	0.53	0.005	1.00	0.00

#### 3.100.2 Detailed Probabilities of GLY100N:

Overall probability: 1.000

Overall confidence: 0.889

#### Inter- and intra-residue probability

Residue	Probability	Confidence
SER99	1.00	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	0.00
SER99	HB2	1.00	0.000	1.00	0.00
SER99	HB3	1.00	0.000	1.00	0.00
SER99	H	1.00	0.000	1.00	0.00
GLY100	HA2	1.00	0.000	1.00	0.00
GLY100	HA3	1.00	0.000	1.00	0.00
GLY100	H	1.00	0.000	1.00	0.00
LEU101	H	1.00	0.000	1.00	0.00

#### 3.100.3 Detailed Probabilities of GLY100HA2:

Overall probability: 0.857

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER99	1.00	1.00
GLY100	1.00	1.00
LEU101	0.50	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	0.012	1.00	0.00
SER99	H	0.68	0.015	1.00	0.00
GLY100	HA2	1.00	0.000	1.00	0.00
GLY100	HA3	1.00	0.000	1.00	0.00
GLY100	H	1.00	0.000	1.00	0.00
LEU101	HA	1.00	0.101	0.00	0.00
LEU101	H	1.00	0.000	1.00	0.00

**3.100.4 Detailed Probabilities of GLY100HA3:**

Overall probability: 0.900

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
SER99	1.00	1.00
GLY100	1.00	1.00
LEU101	0.67	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)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER99	HA	1.00	0.022	1.00	0.00
SER99	HB2	0.53	0.022	1.00	0.00
SER99	HB3	0.62	0.022	1.00	0.00
SER99	H	0.71	0.022	1.00	0.00
GLY100	HA2	1.00	0.000	1.00	0.00
GLY100	HA3	1.00	0.000	1.00	0.00
GLY100	H	1.00	0.000	1.00	0.00
LEU101	HA	1.00	0.194	0.00	0.00
LEU101	H	1.00	0.000	1.00	0.00
LEU101	HG	0.53	0.004	1.00	0.00

## 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	0.00
SER99	HB2	1.00	0.099	0.00	0.00
SER99	HB3	1.00	0.110	0.00	0.00
SER99	H	1.00	0.000	1.00	0.00
GLY100	HA2	1.00	0.000	1.00	0.00
GLY100	HA3	1.00	0.000	1.00	0.00
GLY100	H	1.00	0.000	1.00	0.00
LEU101	H	1.00	0.000	1.00	0.00

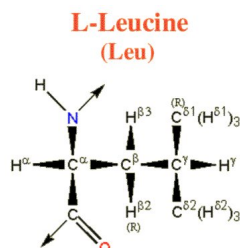


Figure 91: Image from the BMRB

**Residue probability:** 0.969  
**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	0.800	1.000
CB 3.101.2	41.284	42.389	3.750	1.000	1.000
CG 3.101.3	27.245	26.892	3.086	1.000	1.000
CD1 3.101.4	24.911	24.837	3.657	1.000	1.000
CD2 3.101.5	22.335	24.201	3.117	1.000	1.000
N 3.101.6	122.211	121.785	4.943	1.000	1.000
HA 3.101.7	4.361	4.315	0.840	0.800	1.000
HB2 3.101.8	1.415	1.601	0.373	1.000	1.000
HB3 3.101.9	1.297	1.508	0.398	1.000	1.000
HG 3.101.10	1.463	1.510	0.340	1.000	1.000
HD1 3.101.11	0.858	0.739	0.294	1.000	1.000
HD2 3.101.12	0.887	0.727	0.421	1.000	1.000
H 3.101.13	7.308	8.237	0.647	1.000	1.000

**3.101.1 Detailed Probabilities of LEU101CA:**

**Overall probability:** 0.800  
**Overall confidence:** 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLY100	0.00	1.00
LEU101	1.00	1.00
PRO102	0.83	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	0.101	0.00	0.00
GLY100	HA3	1.00	0.194	0.00	0.00
LEU101	HA	1.00	0.000	1.00	0.00
LEU101	HB2	1.00	0.000	1.00	0.00
LEU101	HB3	1.00	0.000	1.00	0.00
LEU101	HG	1.00	0.000	1.00	0.00
LEU101	HD11	0.99	0.000	1.00	0.00
LEU101	HD21	0.99	0.000	1.00	0.00
LEU101	H	1.00	0.000	1.00	0.00
PRO102	HA	1.00	0.147	0.00	0.00
PRO102	HD2	1.00	0.005	1.00	0.00
PRO102	HD3	1.00	0.007	1.00	0.00
PRO102	HB3	0.77	0.001	1.00	0.00
PRO102	HG2	0.91	0.009	1.00	0.00
PRO102	HG3	0.90	0.010	1.00	0.00

**3.101.2 Detailed Probabilities of LEU101CB:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU101	1.00	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	0.000	1.00	0.00
LEU101	HB2	1.00	0.000	1.00	0.00
LEU101	HB3	1.00	0.000	1.00	0.00
LEU101	HG	1.00	0.000	1.00	0.00
LEU101	HD11	1.00	0.000	1.00	0.00
LEU101	HD21	1.00	0.000	1.00	0.00
LEU101	H	1.00	0.000	1.00	0.00
PRO102	HD2	0.99	0.003	1.00	0.00
PRO102	HD3	1.00	0.008	1.00	0.00

**3.101.3 Detailed Probabilities of LEU101CG:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU101	1.00	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	0.000	1.00	0.00
LEU101	HB2	1.00	0.000	1.00	0.00
LEU101	HB3	1.00	0.000	1.00	0.00
LEU101	HG	1.00	0.000	1.00	0.00
LEU101	HD11	1.00	0.000	1.00	0.00
LEU101	HD21	1.00	0.000	1.00	0.00
LEU101	H	1.00	0.000	1.00	0.00

**3.101.4 Detailed Probabilities of LEU101CD1:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU101	1.00	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	0.000	1.00	0.00
LEU101	HB2	1.00	0.000	1.00	0.00
LEU101	HB3	1.00	0.000	1.00	0.00
LEU101	HG	1.00	0.000	1.00	0.00
LEU101	HD11	1.00	0.000	1.00	0.00
LEU101	HD21	1.00	0.000	1.00	0.00
LEU101	H	0.86	0.000	1.00	0.00

**3.101.5 Detailed Probabilities of LEU101CD2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU101	1.00	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	0.000	1.00	0.00
LEU101	HB2	1.00	0.000	1.00	0.00
LEU101	HB3	1.00	0.000	1.00	0.00
LEU101	HG	1.00	0.000	1.00	0.00
LEU101	HD11	1.00	0.000	1.00	0.00
LEU101	HD21	1.00	0.000	1.00	0.00
LEU101	H	0.85	0.000	1.00	0.00

**3.101.6 Detailed Probabilities of LEU101N:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLY100	1.00	1.00
LEU101	1.00	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	0.00
GLY100	HA3	1.00	0.000	1.00	0.00
GLY100	H	1.00	0.000	1.00	0.00
LEU101	HA	1.00	0.000	1.00	0.00
LEU101	HB2	1.00	0.000	1.00	0.00
LEU101	HB3	1.00	0.000	1.00	0.00
LEU101	HG	1.00	0.000	1.00	0.00
LEU101	H	1.00	0.000	1.00	0.00
LEU101	HD11	0.88	0.000	1.00	0.00
LEU101	HD21	0.87	0.000	1.00	0.00
PRO102	HD2	0.99	0.005	1.00	0.00
PRO102	HD3	0.99	0.007	1.00	0.00

**3.101.7 Detailed Probabilities of LEU101HA:**

Overall probability: 0.800

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLY100	0.00	1.00
LEU101	1.00	1.00
PRO102	0.83	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	0.364	0.00	0.00
GLY100	HA3	1.00	0.364	0.00	0.00
LEU101	HA	1.00	0.000	1.00	0.00
LEU101	HB2	1.00	0.000	1.00	0.00
LEU101	HB3	1.00	0.000	1.00	0.00
LEU101	HG	1.00	0.000	1.00	0.00
LEU101	HD11	0.99	0.000	1.00	0.00
LEU101	HD21	0.99	0.000	1.00	0.00
LEU101	H	1.00	0.000	1.00	0.00
PRO102	HA	1.00	0.147	0.00	0.00
PRO102	HD2	1.00	0.000	1.00	0.00
PRO102	HD3	1.00	0.009	1.00	0.00
PRO102	HB3	0.77	0.003	1.00	0.00
PRO102	HG2	0.91	0.001	1.00	0.00
PRO102	HG3	0.90	0.001	1.00	0.00

**3.101.8 Detailed Probabilities of LEU101HB2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU101	1.00	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	0.000	1.00	0.00
LEU101	HB2	1.00	0.000	1.00	0.00
LEU101	HB3	1.00	0.000	1.00	0.00
LEU101	HG	1.00	0.000	1.00	0.00
LEU101	HD11	1.00	0.000	1.00	0.00
LEU101	HD21	1.00	0.000	1.00	0.00
LEU101	H	1.00	0.000	1.00	0.00
PRO102	HD2	0.99	0.007	1.00	0.00
PRO102	HD3	1.00	0.013	1.00	0.00

**3.101.9 Detailed Probabilities of LEU101HB3:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU101	1.00	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**

## 3.101 LEU(101)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU101	HA	1.00	0.000	1.00	0.00
LEU101	HB2	1.00	0.000	1.00	0.00
LEU101	HB3	1.00	0.000	1.00	0.00
LEU101	HG	1.00	0.000	1.00	0.00
LEU101	HD11	1.00	0.000	1.00	0.00
LEU101	HD21	1.00	0.000	1.00	0.00
LEU101	H	1.00	0.000	1.00	0.00
PRO102	HD2	1.00	0.012	1.00	0.00
PRO102	HD3	1.00	0.027	1.00	0.00

## 3.101.10 Detailed Probabilities of LEU101HG:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
LEU101	1.00	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	0.000	1.00	0.00
LEU101	HB2	1.00	0.000	1.00	0.00
LEU101	HB3	1.00	0.000	1.00	0.00
LEU101	HG	1.00	0.000	1.00	0.00
LEU101	HD11	1.00	0.000	1.00	0.00
LEU101	HD21	1.00	0.000	1.00	0.00
LEU101	H	1.00	0.000	1.00	0.00

## 3.101.11 Detailed Probabilities of LEU101HD11:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
LEU101	1.00	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	0.000	1.00	0.00
LEU101	HB2	1.00	0.000	1.00	0.00
LEU101	HB3	1.00	0.000	1.00	0.00
LEU101	HG	1.00	0.000	1.00	0.00
LEU101	HD11	1.00	0.000	1.00	0.00
LEU101	HD21	1.00	0.000	1.00	0.00
LEU101	H	0.86	0.000	1.00	0.00

**3.101.12 Detailed Probabilities of LEU101HD21:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU101	1.00	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	0.000	1.00	0.00
LEU101	HB2	1.00	0.000	1.00	0.00
LEU101	HB3	1.00	0.000	1.00	0.00
LEU101	HG	1.00	0.000	1.00	0.00
LEU101	HD11	1.00	0.000	1.00	0.00
LEU101	HD21	1.00	0.000	1.00	0.00
LEU101	H	0.85	0.000	1.00	0.00

**3.101.13 Detailed Probabilities of LEU101H:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLY100	1.00	1.00
LEU101	1.00	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	0.00
GLY100	HA3	1.00	0.000	1.00	0.00
GLY100	H	1.00	0.000	1.00	0.00
LEU101	HA	1.00	0.000	1.00	0.00
LEU101	HB2	1.00	0.000	1.00	0.00
LEU101	HB3	1.00	0.000	1.00	0.00
LEU101	HG	1.00	0.000	1.00	0.00
LEU101	H	1.00	0.000	1.00	0.00
LEU101	HD11	0.88	0.000	1.00	0.00
LEU101	HD21	0.87	0.000	1.00	0.00
PRO102	HD2	0.99	0.003	1.00	0.00
PRO102	HD3	0.99	0.003	1.00	0.00

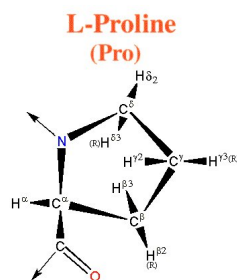
**3.102 PRO(102)**

Figure 92: Image from the BMRB

**Residue probability:** 0.937**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	0.636	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	1.000	1.000
CD 3.102.4	50.118	49.797	3.175	1.000	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	1.000	1.000
HB3 3.102.7	2.325	2.052	0.596	1.000	1.000
HG2 3.102.8	2.051	1.927	0.364	1.000	1.000
HG3 3.102.9	2.050	1.907	0.417	1.000	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	0.923	1.000

**3.102.1 Detailed Probabilities of PRO102CA:****Overall probability:** 0.636**Overall confidence:** 1.000**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU101	0.00	1.00
PRO102	0.71	1.00
LEU103	0.67	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	0.147	0.00	0.00
PRO102	HA	1.00	0.000	1.00	0.00
PRO102	HB2	1.00	0.000	1.00	0.00
PRO102	HB3	1.00	0.000	1.00	0.00
PRO102	HG2	1.00	0.000	1.00	0.00
PRO102	HG3	1.00	0.000	1.00	0.00
PRO102	HD2	1.00	0.710	0.00	0.00
PRO102	HD3	1.00	0.924	0.00	0.00
LEU103	HA	1.00	0.519	0.00	0.00
LEU103	H	1.00	0.000	1.00	0.00
LEU103	HB2	0.65	0.020	1.00	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)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PRO102	HA	1.00	0.000	1.00	0.00
PRO102	HB2	1.00	0.000	1.00	0.00
PRO102	HB3	1.00	0.000	1.00	0.00
PRO102	HG2	1.00	0.000	1.00	0.00
PRO102	HG3	1.00	0.000	1.00	0.00
PRO102	HD2	1.00	0.000	1.00	0.00
PRO102	HD3	1.00	0.000	1.00	0.00
LEU103	H	1.00	0.000	1.00	0.00

## 3.102.3 Detailed Probabilities of PRO102CG:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
PRO102	1.00	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	0.000	1.00	0.00
PRO102	HB2	1.00	0.000	1.00	0.00
PRO102	HB3	1.00	0.000	1.00	0.00
PRO102	HG2	1.00	0.000	1.00	0.00
PRO102	HG3	1.00	0.000	1.00	0.00
PRO102	HD2	1.00	0.000	1.00	0.00
PRO102	HD3	1.00	0.000	1.00	0.00

## 3.102.4 Detailed Probabilities of PRO102CD:

Overall probability: 1.000

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
LEU101	1.00	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	0.000	1.00	0.00
LEU101	HB2	0.99	0.007	1.00	0.00
LEU101	HB3	1.00	0.012	1.00	0.00
LEU101	H	0.99	0.003	1.00	0.00
LEU101	HD11	0.63	0.015	1.00	0.00
LEU101	HD21	0.76	0.014	1.00	0.00
PRO102	HA	1.00	0.000	1.00	0.00
PRO102	HB2	1.00	0.000	1.00	0.00
PRO102	HB3	1.00	0.000	1.00	0.00
PRO102	HG2	1.00	0.000	1.00	0.00
PRO102	HG3	1.00	0.000	1.00	0.00
PRO102	HD2	1.00	0.000	1.00	0.00
PRO102	HD3	1.00	0.000	1.00	0.00

**3.102.5 Detailed Probabilities of PRO102HA:**

Overall probability: 0.818

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU101	0.00	1.00
PRO102	1.00	1.00
LEU103	0.67	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	0.147	0.00	0.00
PRO102	HA	1.00	0.000	1.00	0.00
PRO102	HB2	1.00	0.000	1.00	0.00
PRO102	HB3	1.00	0.000	1.00	0.00
PRO102	HG2	1.00	0.000	1.00	0.00
PRO102	HG3	1.00	0.000	1.00	0.00
PRO102	HD2	1.00	0.000	1.00	0.00
PRO102	HD3	1.00	0.000	1.00	0.00
LEU103	HA	1.00	0.315	0.00	0.00
LEU103	H	1.00	0.000	1.00	0.00
LEU103	HB2	0.65	0.012	1.00	0.00

**3.102.6 Detailed Probabilities of PRO102HB2:**

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
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	0.000	1.00	0.00
PRO102	HB2	1.00	0.000	1.00	0.00
PRO102	HB3	1.00	0.000	1.00	0.00
PRO102	HG2	1.00	0.000	1.00	0.00
PRO102	HG3	1.00	0.000	1.00	0.00
PRO102	HD2	1.00	0.000	1.00	0.00
PRO102	HD3	1.00	0.000	1.00	0.00
LEU103	HA	0.99	0.013	1.00	0.00
LEU103	H	1.00	0.000	1.00	0.00

**3.102.7 Detailed Probabilities of PRO102HB3:**

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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PRO102	HA	1.00	0.000	1.00	0.00
PRO102	HB2	1.00	0.000	1.00	0.00
PRO102	HB3	1.00	0.000	1.00	0.00
PRO102	HG2	1.00	0.000	1.00	0.00
PRO102	HG3	1.00	0.000	1.00	0.00
PRO102	HD2	1.00	0.000	1.00	0.00
PRO102	HD3	1.00	0.000	1.00	0.00
LEU103	H	1.00	0.000	1.00	0.00

**3.102.8 Detailed Probabilities of PRO102HG2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO102	1.00	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	0.000	1.00	0.00
PRO102	HB2	1.00	0.000	1.00	0.00
PRO102	HB3	1.00	0.000	1.00	0.00
PRO102	HG2	1.00	0.000	1.00	0.00
PRO102	HG3	1.00	0.000	1.00	0.00
PRO102	HD2	1.00	0.000	1.00	0.00
PRO102	HD3	1.00	0.000	1.00	0.00

**3.102.9 Detailed Probabilities of PRO102HG3:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO102	1.00	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	0.000	1.00	0.00
PRO102	HB2	1.00	0.000	1.00	0.00
PRO102	HB3	1.00	0.000	1.00	0.00
PRO102	HG2	1.00	0.000	1.00	0.00
PRO102	HG3	1.00	0.000	1.00	0.00
PRO102	HD2	1.00	0.000	1.00	0.00
PRO102	HD3	1.00	0.000	1.00	0.00

**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	0.005	1.00	0.00
LEU101	HB2	0.99	0.003	1.00	0.00
LEU101	HB3	1.00	0.001	1.00	0.00
LEU101	H	0.99	0.005	1.00	0.00
LEU101	HG	0.94	0.002	1.00	0.00
LEU101	HD11	0.63	0.005	1.00	0.00
LEU101	HD21	0.76	0.006	1.00	0.00
PRO102	HA	1.00	0.710	0.00	0.00
PRO102	HB2	1.00	0.000	1.00	0.00
PRO102	HB3	1.00	0.000	1.00	0.00
PRO102	HG2	1.00	0.000	1.00	0.00
PRO102	HG3	1.00	0.000	1.00	0.00
PRO102	HD2	1.00	0.000	1.00	0.00
PRO102	HD3	1.00	0.000	1.00	0.00

**3.102.11 Detailed Probabilities of PRO102HD3:**

Overall probability: 0.923

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
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	0.00
LEU101	HB2	1.00	0.008	1.00	0.00
LEU101	HB3	1.00	0.015	1.00	0.00
LEU101	H	0.99	0.007	1.00	0.00
LEU101	HG	0.83	0.011	1.00	0.00
LEU101	HD21	0.59	0.007	1.00	0.00
PRO102	HA	1.00	0.924	0.00	0.00
PRO102	HB2	1.00	0.000	1.00	0.00
PRO102	HB3	1.00	0.000	1.00	0.00
PRO102	HG2	1.00	0.000	1.00	0.00
PRO102	HG3	1.00	0.000	1.00	0.00
PRO102	HD2	1.00	0.000	1.00	0.00
PRO102	HD3	1.00	0.000	1.00	0.00

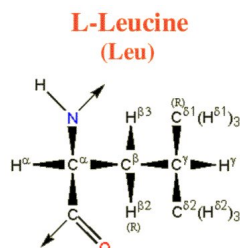


Figure 93: Image from the BMRB

**Residue probability:** 0.967  
**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	0.818	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	1.000	1.000
CD2 3.103.5	25.933	24.201	3.117	1.000	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	0.751	1.000
HB2 3.103.8	1.693	1.601	0.373	1.000	1.000
HB3 3.103.9	1.554	1.508	0.398	1.000	1.000
HG 3.103.10	1.573	1.510	0.340	1.000	1.000
HD1 3.103.11	0.548	0.739	0.294	1.000	1.000
HD2 3.103.12	0.518	0.727	0.421	1.000	1.000
H 3.103.13	8.358	8.237	0.647	1.000	1.000

**3.103.1 Detailed Probabilities of LEU103CA:**

**Overall probability:** 0.818  
**Overall confidence:** 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO102	0.50	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	0.315	0.00	0.00
PRO102	HB2	0.99	0.013	1.00	0.00
LEU103	HA	1.00	0.000	1.00	0.00
LEU103	HB2	1.00	0.000	1.00	0.00
LEU103	HB3	1.00	0.000	1.00	0.00
LEU103	HG	1.00	0.000	1.00	0.00
LEU103	HD11	0.99	0.000	1.00	0.00
LEU103	HD21	0.99	0.000	1.00	0.00
LEU103	H	1.00	0.000	1.00	0.00
VAL104	HA	1.00	0.725	0.00	0.00
VAL104	H	1.00	0.000	1.00	0.00

**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)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU103	HA	1.00	0.000	1.00	0.00
LEU103	HB2	1.00	0.000	1.00	0.00
LEU103	HB3	1.00	0.000	1.00	0.00
LEU103	HG	1.00	0.000	1.00	0.00
LEU103	HD11	1.00	0.000	1.00	0.00
LEU103	HD21	1.00	0.000	1.00	0.00
LEU103	H	1.00	0.000	1.00	0.00
VAL104	H	1.00	0.000	1.00	0.00

#### 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	0.00
LEU103	HB2	1.00	0.000	1.00	0.00
LEU103	HB3	1.00	0.000	1.00	0.00
LEU103	HG	1.00	0.000	1.00	0.00
LEU103	HD11	1.00	0.000	1.00	0.00
LEU103	HD21	1.00	0.000	1.00	0.00
LEU103	H	1.00	0.000	1.00	0.00
VAL104	H	0.98	0.000	1.00	0.00

#### 3.103.4 Detailed Probabilities of LEU103CD1:

Overall probability: 1.000

Overall confidence: 1.000

##### Inter- and intra-residue probability

Residue	Probability	Confidence
LEU103	1.00	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	0.000	1.00	0.00
LEU103	HB2	1.00	0.000	1.00	0.00
LEU103	HB3	1.00	0.000	1.00	0.00
LEU103	HG	1.00	0.000	1.00	0.00
LEU103	HD11	1.00	0.000	1.00	0.00
LEU103	HD21	1.00	0.000	1.00	0.00
LEU103	H	0.86	0.000	1.00	0.00

**3.103.5 Detailed Probabilities of LEU103CD2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU103	1.00	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	0.000	1.00	0.00
LEU103	HB2	1.00	0.000	1.00	0.00
LEU103	HB3	1.00	0.000	1.00	0.00
LEU103	HG	1.00	0.000	1.00	0.00
LEU103	HD11	1.00	0.000	1.00	0.00
LEU103	HD21	1.00	0.000	1.00	0.00
LEU103	H	0.85	0.000	1.00	0.00

**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	0.00
PRO102	HB2	1.00	0.000	1.00	0.00
PRO102	HB3	1.00	0.000	1.00	0.00
PRO102	HG2	0.91	0.000	1.00	0.00
PRO102	HG3	0.74	0.000	1.00	0.00
LEU103	HA	1.00	0.000	1.00	0.00
LEU103	HB2	1.00	0.000	1.00	0.00
LEU103	HB3	1.00	0.000	1.00	0.00
LEU103	HG	1.00	0.000	1.00	0.00
LEU103	H	1.00	0.000	1.00	0.00
LEU103	HD11	0.88	0.000	1.00	0.00
LEU103	HD21	0.87	0.000	1.00	0.00
VAL104	H	1.00	0.000	1.00	0.00

**3.103.7 Detailed Probabilities of LEU103HA:**

Overall probability: 0.751

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
PRO102	0.34	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	0.519	0.00	0.00
PRO102	HB2	0.99	0.062	0.01	0.00
PRO102	HG2	0.61	0.002	1.00	0.00
LEU103	HA	1.00	0.000	1.00	0.00
LEU103	HB2	1.00	0.000	1.00	0.00
LEU103	HB3	1.00	0.000	1.00	0.00
LEU103	HG	1.00	0.000	1.00	0.00
LEU103	HD11	0.99	0.000	1.00	0.00
LEU103	HD21	0.99	0.000	1.00	0.00
LEU103	H	1.00	0.000	1.00	0.00
VAL104	HA	1.00	0.151	0.00	0.00
VAL104	H	1.00	0.000	1.00	0.00

**3.103.8 Detailed Probabilities of LEU103HB2:**

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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU103	HA	1.00	0.000	1.00	0.00
LEU103	HB2	1.00	0.000	1.00	0.00
LEU103	HB3	1.00	0.000	1.00	0.00
LEU103	HG	1.00	0.000	1.00	0.00
LEU103	HD11	1.00	0.000	1.00	0.00
LEU103	HD21	1.00	0.000	1.00	0.00
LEU103	H	1.00	0.000	1.00	0.00
VAL104	H	1.00	0.000	1.00	0.00

**3.103.9 Detailed Probabilities of LEU103HB3:**

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
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	0.000	1.00	0.00
LEU103	HB2	1.00	0.000	1.00	0.00
LEU103	HB3	1.00	0.000	1.00	0.00
LEU103	HG	1.00	0.000	1.00	0.00
LEU103	HD11	1.00	0.000	1.00	0.00
LEU103	HD21	1.00	0.000	1.00	0.00
LEU103	H	1.00	0.000	1.00	0.00
VAL104	H	1.00	0.000	1.00	0.00

**3.103.10 Detailed Probabilities of LEU103HG:**

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	0.00
LEU103	HB2	1.00	0.000	1.00	0.00
LEU103	HB3	1.00	0.000	1.00	0.00
LEU103	HG	1.00	0.000	1.00	0.00
LEU103	HD11	1.00	0.000	1.00	0.00
LEU103	HD21	1.00	0.000	1.00	0.00
LEU103	H	1.00	0.000	1.00	0.00
VAL104	H	0.98	0.000	1.00	0.00

**3.103.11 Detailed Probabilities of LEU103HD11:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU103	1.00	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	0.000	1.00	0.00
LEU103	HB2	1.00	0.000	1.00	0.00
LEU103	HB3	1.00	0.000	1.00	0.00
LEU103	HG	1.00	0.000	1.00	0.00
LEU103	HD11	1.00	0.000	1.00	0.00
LEU103	HD21	1.00	0.000	1.00	0.00
LEU103	H	0.86	0.000	1.00	0.00

**3.103.12 Detailed Probabilities of LEU103HD21:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU103	1.00	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	0.000	1.00	0.00
LEU103	HB2	1.00	0.000	1.00	0.00
LEU103	HB3	1.00	0.000	1.00	0.00
LEU103	HG	1.00	0.000	1.00	0.00
LEU103	HD11	1.00	0.000	1.00	0.00
LEU103	HD21	1.00	0.000	1.00	0.00
LEU103	H	0.85	0.000	1.00	0.00

**3.103.13 Detailed Probabilities of LEU103H:**

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	0.00
PRO102	HB2	1.00	0.000	1.00	0.00
PRO102	HB3	1.00	0.000	1.00	0.00
PRO102	HG2	0.91	0.000	1.00	0.00
PRO102	HG3	0.74	0.000	1.00	0.00
LEU103	HA	1.00	0.000	1.00	0.00
LEU103	HB2	1.00	0.000	1.00	0.00
LEU103	HB3	1.00	0.000	1.00	0.00
LEU103	HG	1.00	0.000	1.00	0.00
LEU103	H	1.00	0.000	1.00	0.00
LEU103	HD11	0.88	0.000	1.00	0.00
LEU103	HD21	0.87	0.000	1.00	0.00
VAL104	H	1.00	0.000	1.00	0.00

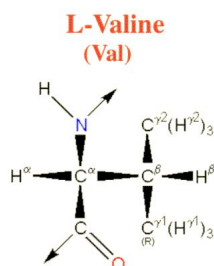


Figure 94: Image from the BMRB

Residue probability: 0.950  
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	0.750	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	1.000	1.000
CG2 3.104.4	20.796	21.368	2.801	1.000	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	0.750	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	1.000	1.000
HG2 3.104.9	0.998	0.803	0.504	1.000	1.000
H 3.104.10	7.758	8.311	0.669	1.000	1.000

**3.104.1 Detailed Probabilities of VAL104CA:**

Overall probability: 0.750  
Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU103	0.00	1.00
VAL104	1.00	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	0.151	0.00	0.00
VAL104	HA	1.00	0.000	1.00	0.00
VAL104	HB	1.00	0.000	1.00	0.00
VAL104	HG11	1.00	0.000	1.00	0.00
VAL104	HG21	1.00	0.000	1.00	0.00
VAL104	H	1.00	0.000	1.00	0.00
THR105	HA	1.00	0.069	0.00	0.00
THR105	H	1.00	0.000	1.00	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	0.000	1.00	0.00
VAL104	HB	1.00	0.000	1.00	0.00
VAL104	HG11	1.00	0.000	1.00	0.00
VAL104	HG21	1.00	0.000	1.00	0.00
VAL104	H	1.00	0.000	1.00	0.00
THR105	H	1.00	0.000	1.00	0.00

**3.104.3 Detailed Probabilities of VAL104CG1:**

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
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	0.000	1.00	0.00
VAL104	HB	1.00	0.000	1.00	0.00
VAL104	HG11	1.00	0.000	1.00	0.00
VAL104	HG21	1.00	0.000	1.00	0.00
VAL104	H	1.00	0.000	1.00	0.00
THR105	H	0.97	0.000	1.00	0.00
THR105	HA	0.52	0.012	1.00	0.00

**3.104.4 Detailed Probabilities of VAL104CG2:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL104	1.00	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	0.000	1.00	0.00
VAL104	HB	1.00	0.000	1.00	0.00
VAL104	HG11	1.00	0.000	1.00	0.00
VAL104	HG21	1.00	0.000	1.00	0.00
VAL104	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
LEU103	HB2	1.00	0.000	1.00	0.00
LEU103	HB3	1.00	0.000	1.00	0.00
LEU103	HG	0.98	0.000	1.00	0.00
LEU103	H	1.00	0.000	1.00	0.00
LEU103	HD11	0.55	0.000	1.00	0.00
LEU103	HD21	0.58	0.000	1.00	0.00
VAL104	HA	1.00	0.000	1.00	0.00
VAL104	HB	1.00	0.000	1.00	0.00
VAL104	HG11	1.00	0.000	1.00	0.00
VAL104	HG21	1.00	0.000	1.00	0.00
VAL104	H	1.00	0.000	1.00	0.00
THR105	H	1.00	0.000	1.00	0.00

**3.104.6 Detailed Probabilities of VAL104HA:**

Overall probability: 0.750

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
LEU103	0.00	1.00
VAL104	1.00	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	0.725	0.00	0.00
VAL104	HA	1.00	0.000	1.00	0.00
VAL104	HB	1.00	0.000	1.00	0.00
VAL104	HG11	1.00	0.000	1.00	0.00
VAL104	HG21	1.00	0.000	1.00	0.00
VAL104	H	1.00	0.000	1.00	0.00
THR105	HA	1.00	0.479	0.00	0.00
THR105	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
VAL104	HB	1.00	0.000	1.00	0.00
VAL104	HG11	1.00	0.000	1.00	0.00
VAL104	HG21	1.00	0.000	1.00	0.00
VAL104	H	1.00	0.000	1.00	0.00
THR105	H	1.00	0.000	1.00	0.00

**3.104.8 Detailed Probabilities of VAL104HG11:**

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
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	0.000	1.00	0.00
VAL104	HB	1.00	0.000	1.00	0.00
VAL104	HG11	1.00	0.000	1.00	0.00
VAL104	HG21	1.00	0.000	1.00	0.00
VAL104	H	1.00	0.000	1.00	0.00
THR105	H	0.97	0.000	1.00	0.00
THR105	HA	0.52	0.017	1.00	0.00

**3.104.9 Detailed Probabilities of VAL104HG21:**

Overall probability: 1.000

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
VAL104	1.00	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	0.000	1.00	0.00
VAL104	HB	1.00	0.000	1.00	0.00
VAL104	HG11	1.00	0.000	1.00	0.00
VAL104	HG21	1.00	0.000	1.00	0.00
VAL104	H	1.00	0.000	1.00	0.00

**3.104.10 Detailed Probabilities of VAL104H:**

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	0.000	1.00	0.00
LEU103	HB2	1.00	0.000	1.00	0.00
LEU103	HB3	1.00	0.000	1.00	0.00
LEU103	HG	0.98	0.000	1.00	0.00
LEU103	H	1.00	0.000	1.00	0.00
LEU103	HD11	0.55	0.000	1.00	0.00
LEU103	HD21	0.58	0.000	1.00	0.00
VAL104	HA	1.00	0.000	1.00	0.00
VAL104	HB	1.00	0.000	1.00	0.00
VAL104	HG11	1.00	0.000	1.00	0.00
VAL104	HG21	1.00	0.000	1.00	0.00
VAL104	H	1.00	0.000	1.00	0.00
THR105	H	1.00	0.000	1.00	0.00

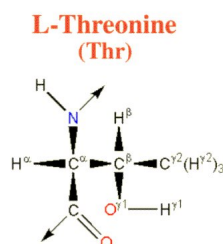
**3.105 THR(105)**

Figure 95: Image from the BMRB

Residue probability: 0.970

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	0.875	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	1.000	0.900
HG1	NA	—	—	0.000	0.000

**3.105.1 Detailed Probabilities of THR105CA:**

Overall probability: 0.875

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	0.479	0.00	0.00
VAL104	HG11	0.54	0.017	1.00	0.00
THR105	HA	1.00	0.000	1.00	0.00
THR105	HB	1.00	0.000	1.00	0.00
THR105	HG21	1.00	0.000	1.00	0.00
THR105	H	1.00	0.000	1.00	0.00
GLU106	HA	1.00	0.020	1.00	0.00
GLU106	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
THR105	HB	1.00	0.000	1.00	0.00
THR105	HG21	1.00	0.000	1.00	0.00
THR105	H	1.00	0.000	1.00	0.00
GLU106	H	1.00	0.000	1.00	0.00
GLU106	HA	0.79	0.020	1.00	0.00

**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	0.000	1.00	0.00
THR105	HB	1.00	0.000	1.00	0.00
THR105	HG21	1.00	0.000	1.00	0.00
THR105	H	1.00	0.000	1.00	0.00
GLU106	H	0.95	0.000	1.00	0.00

**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	0.000	1.00	0.00
VAL104	HB	1.00	0.000	1.00	0.00
VAL104	HG11	0.97	0.000	1.00	0.00
VAL104	H	1.00	0.000	1.00	0.00
VAL104	HG21	0.94	0.000	1.00	0.00
THR105	HA	1.00	0.000	1.00	0.00
THR105	HB	1.00	0.000	1.00	0.00
THR105	HG21	1.00	0.000	1.00	0.00
THR105	H	1.00	0.000	1.00	0.00
GLU106	H	1.00	0.000	1.00	0.00
GLU106	HA	0.82	0.020	1.00	0.00

## 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	HG11	0.54	0.012	1.00	0.00
THR105	HA	1.00	0.000	1.00	0.00
THR105	HB	1.00	0.000	1.00	0.00
THR105	HG21	1.00	0.000	1.00	0.00
THR105	H	1.00	0.000	1.00	0.00
GLU106	HA	1.00	0.020	1.00	0.00
GLU106	H	1.00	0.000	1.00	0.00
GLU106	HB2	0.56	0.020	1.00	0.00

**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	0.000	1.00	0.00
THR105	HB	1.00	0.000	1.00	0.00
THR105	HG21	1.00	0.000	1.00	0.00
THR105	H	1.00	0.000	1.00	0.00
GLU106	H	1.00	0.000	1.00	0.00

**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	0.000	1.00	0.00
THR105	HB	1.00	0.000	1.00	0.00
THR105	HG21	1.00	0.000	1.00	0.00
THR105	H	1.00	0.000	1.00	0.00
GLU106	H	0.95	0.000	1.00	0.00

**3.105.8 Detailed Probabilities of THR105H:**

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**

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL104	HA	1.00	0.000	1.00	0.00
VAL104	HB	1.00	0.000	1.00	0.00
VAL104	HG11	0.97	0.000	1.00	0.00
VAL104	H	1.00	0.000	1.00	0.00
VAL104	HG21	0.94	0.000	1.00	0.00
THR105	HA	1.00	0.000	1.00	0.00
THR105	HB	1.00	0.000	1.00	0.00
THR105	HG21	1.00	0.000	1.00	0.00
THR105	H	1.00	0.000	1.00	0.00
GLU106	H	1.00	0.000	1.00	0.00

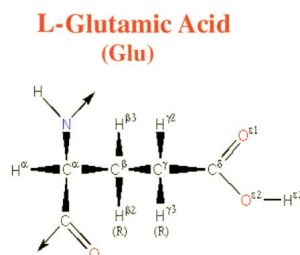
**3.106 GLU(106)**

Figure 96: Image from the BMRB

Residue probability: 0.980

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	0.889	1.000
CB 3.106.2	30.613	30.185	4.018	1.000	0.875
CG 3.106.3	36.010	36.085	1.533	1.000	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	0.909	1.000
HB2 3.106.6	2.154	2.021	0.233	1.000	0.875
HB3 3.106.7	1.949	1.994	0.244	1.000	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	1.000	0.917
HE2	NA	—	—	0.000	0.000

**3.106.1 Detailed Probabilities of GLU106CA:**

Overall probability: 0.889

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
THR105	1.00	1.00
GLU106	1.00	1.00
GLU107	0.50	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	0.020	1.00	0.00
GLU106	HA	1.00	0.000	1.00	0.00
GLU106	HB2	1.00	0.000	1.00	0.00
GLU106	HB3	1.00	0.000	1.00	0.00
GLU106	HG2	1.00	0.000	1.00	0.00
GLU106	HG3	1.00	0.000	1.00	0.00
GLU106	H	1.00	0.000	1.00	0.00
GLU107	HA	1.00	0.290	0.00	0.00
GLU107	H	1.00	0.000	1.00	0.00

**3.106.2 Detailed Probabilities of GLU106CB:**

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
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	0.000	1.00	0.00
GLU106	HB2	1.00	0.000	1.00	0.00
GLU106	HB3	1.00	0.000	1.00	0.00
GLU106	HG2	1.00	0.000	1.00	0.00
GLU106	HG3	1.00	0.000	1.00	0.00
GLU106	H	1.00	0.000	1.00	0.00
GLU107	H	1.00	0.000	1.00	0.00

**3.106.3 Detailed Probabilities of GLU106CG:**

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	0.00
GLU106	HB2	1.00	0.000	1.00	0.00
GLU106	HB3	1.00	0.000	1.00	0.00
GLU106	HG2	1.00	0.000	1.00	0.00
GLU106	HG3	1.00	0.000	1.00	0.00
GLU106	H	1.00	0.000	1.00	0.00
GLU107	H	0.98	0.000	1.00	0.00

**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**

## 3.106 GLU(106)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR105	HA	1.00	0.000	1.00	0.00
THR105	HB	1.00	0.000	1.00	0.00
THR105	HG21	0.95	0.000	1.00	0.00
THR105	H	1.00	0.000	1.00	0.00
GLU106	HA	1.00	0.000	1.00	0.00
GLU106	HB2	1.00	0.000	1.00	0.00
GLU106	HB3	1.00	0.000	1.00	0.00
GLU106	HG2	1.00	0.000	1.00	0.00
GLU106	HG3	1.00	0.000	1.00	0.00
GLU106	H	1.00	0.000	1.00	0.00
GLU107	H	1.00	0.000	1.00	0.00

## 3.106.5 Detailed Probabilities of GLU106HA:

Overall probability: 0.909

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
THR105	1.00	1.00
GLU106	1.00	1.00
GLU107	0.50	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	0.020	1.00	0.00
THR105	HB	0.79	0.020	1.00	0.00
THR105	H	0.82	0.020	1.00	0.00
GLU106	HA	1.00	0.000	1.00	0.00
GLU106	HB2	1.00	0.000	1.00	0.00
GLU106	HB3	1.00	0.000	1.00	0.00
GLU106	HG2	1.00	0.000	1.00	0.00
GLU106	HG3	1.00	0.000	1.00	0.00
GLU106	H	1.00	0.000	1.00	0.00
GLU107	HA	1.00	0.304	0.00	0.00
GLU107	H	1.00	0.000	1.00	0.00

**3.106.6 Detailed Probabilities of GLU106HB2:**

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
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	0.000	1.00	0.00
GLU106	HB2	1.00	0.000	1.00	0.00
GLU106	HB3	1.00	0.000	1.00	0.00
GLU106	HG2	1.00	0.000	1.00	0.00
GLU106	HG3	1.00	0.000	1.00	0.00
GLU106	H	1.00	0.000	1.00	0.00
GLU107	H	1.00	0.000	1.00	0.00

**3.106.7 Detailed Probabilities of GLU106HB3:**

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
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	0.00
GLU106	HB2	1.00	0.000	1.00	0.00
GLU106	HB3	1.00	0.000	1.00	0.00
GLU106	HG2	1.00	0.000	1.00	0.00
GLU106	HG3	1.00	0.000	1.00	0.00
GLU106	H	1.00	0.000	1.00	0.00
GLU107	H	1.00	0.000	1.00	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	0.00
GLU106	HB2	1.00	0.000	1.00	0.00
GLU106	HB3	1.00	0.000	1.00	0.00
GLU106	HG2	1.00	0.000	1.00	0.00
GLU106	HG3	1.00	0.000	1.00	0.00
GLU106	H	1.00	0.000	1.00	0.00
GLU107	H	0.98	0.000	1.00	0.00

**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	0.000	1.00	0.00
GLU106	HB2	1.00	0.000	1.00	0.00
GLU106	HB3	1.00	0.000	1.00	0.00
GLU106	HG2	1.00	0.000	1.00	0.00
GLU106	HG3	1.00	0.000	1.00	0.00
GLU106	H	1.00	0.000	1.00	0.00
GLU107	H	0.97	0.000	1.00	0.00

**3.106.10 Detailed Probabilities of GLU106H:**

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**

## 3.106 GLU(106)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR105	HA	1.00	0.000	1.00	0.00
THR105	HB	1.00	0.000	1.00	0.00
THR105	HG21	0.95	0.000	1.00	0.00
THR105	H	1.00	0.000	1.00	0.00
GLU106	HA	1.00	0.000	1.00	0.00
GLU106	HB2	1.00	0.000	1.00	0.00
GLU106	HB3	1.00	0.000	1.00	0.00
GLU106	HG2	1.00	0.000	1.00	0.00
GLU106	HG3	1.00	0.000	1.00	0.00
GLU106	H	1.00	0.000	1.00	0.00
GLU107	H	1.00	0.000	1.00	0.00

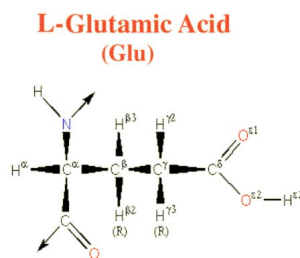
**3.107 GLU(107)**

Figure 97: Image from the BMRB

Residue probability: 0.971

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	0.857	1.000
CB 3.107.2	31.124	30.185	4.018	1.000	0.857
CG 3.107.3	36.717	36.085	1.533	1.000	0.857
N 3.107.4	126.458	120.574	4.837	1.000	1.000
HA 3.107.5	4.115	4.245	0.429	0.857	1.000
HB2 3.107.6	1.903	2.021	0.233	1.000	0.857
HB3 3.107.7	2.067	1.994	0.244	1.000	0.857
HG2 3.107.8	2.220	2.258	0.226	1.000	0.857
HG3 3.107.9	2.218	2.233	0.232	1.000	0.857
H 3.107.10	8.130	8.332	0.601	1.000	1.000
HE2	NA	—	—	0.000	0.000

**3.107.1 Detailed Probabilities of GLU107CA:**

Overall probability: 0.857

Overall confidence: 1.000

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU106	0.00	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	0.304	0.00	0.00
GLU107	HA	1.00	0.000	1.00	0.00
GLU107	HB2	1.00	0.000	1.00	0.00
GLU107	HB3	1.00	0.000	1.00	0.00
GLU107	HG2	1.00	0.000	1.00	0.00
GLU107	HG3	1.00	0.000	1.00	0.00
GLU107	H	1.00	0.000	1.00	0.00

**3.107.2 Detailed Probabilities of GLU107CB:**

Overall probability: 1.000

Overall confidence: 0.857

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU107	1.00	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	0.000	1.00	0.00
GLU107	HB2	1.00	0.000	1.00	0.00
GLU107	HB3	1.00	0.000	1.00	0.00
GLU107	HG2	1.00	0.000	1.00	0.00
GLU107	HG3	1.00	0.000	1.00	0.00
GLU107	H	1.00	0.005	1.00	0.00

**3.107.3 Detailed Probabilities of GLU107CG:**

Overall probability: 1.000

Overall confidence: 0.857

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU107	1.00	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	0.000	1.00	0.00
GLU107	HB2	1.00	0.000	1.00	0.00
GLU107	HB3	1.00	0.000	1.00	0.00
GLU107	HG2	1.00	0.000	1.00	0.00
GLU107	HG3	1.00	0.000	1.00	0.00
GLU107	H	1.00	0.000	1.00	0.00

**3.107.4 Detailed Probabilities of GLU107N:**

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
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**

## 3.107 GLU(107)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU106	HA	1.00	0.000	1.00	0.00
GLU106	HB2	1.00	0.000	1.00	0.00
GLU106	HB3	1.00	0.000	1.00	0.00
GLU106	HG2	0.98	0.000	1.00	0.00
GLU106	HG3	0.97	0.000	1.00	0.00
GLU106	H	1.00	0.000	1.00	0.00
GLU107	HA	1.00	0.000	1.00	0.00
GLU107	HB2	1.00	0.000	1.00	0.00
GLU107	HB3	1.00	0.000	1.00	0.00
GLU107	HG2	1.00	0.000	1.00	0.00
GLU107	HG3	1.00	0.000	1.00	0.00
GLU107	H	1.00	0.000	1.00	0.00

## 3.107.5 Detailed Probabilities of GLU107HA:

Overall probability: 0.857

Overall confidence: 1.000

## Inter- and intra-residue probability

Residue	Probability	Confidence
GLU106	0.00	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	0.290	0.00	0.00
GLU107	HA	1.00	0.000	1.00	0.00
GLU107	HB2	1.00	0.000	1.00	0.00
GLU107	HB3	1.00	0.000	1.00	0.00
GLU107	HG2	1.00	0.000	1.00	0.00
GLU107	HG3	1.00	0.000	1.00	0.00
GLU107	H	1.00	0.000	1.00	0.00

## 3.107.6 Detailed Probabilities of GLU107HB2:

Overall probability: 1.000

Overall confidence: 0.857

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU107	1.00	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	0.000	1.00	0.00
GLU107	HB2	1.00	0.000	1.00	0.00
GLU107	HB3	1.00	0.000	1.00	0.00
GLU107	HG2	1.00	0.000	1.00	0.00
GLU107	HG3	1.00	0.000	1.00	0.00
GLU107	H	1.00	0.000	1.00	0.00

**3.107.7 Detailed Probabilities of GLU107HB3:**

Overall probability: 1.000

Overall confidence: 0.857

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU107	1.00	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	0.000	1.00	0.00
GLU107	HB2	1.00	0.000	1.00	0.00
GLU107	HB3	1.00	0.000	1.00	0.00
GLU107	HG2	1.00	0.000	1.00	0.00
GLU107	HG3	1.00	0.000	1.00	0.00
GLU107	H	1.00	0.000	1.00	0.00

**3.107.8 Detailed Probabilities of GLU107HG2:**

Overall probability: 1.000

Overall confidence: 0.857

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU107	1.00	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	0.000	1.00	0.00
GLU107	HB2	1.00	0.000	1.00	0.00
GLU107	HB3	1.00	0.000	1.00	0.00
GLU107	HG2	1.00	0.000	1.00	0.00
GLU107	HG3	1.00	0.000	1.00	0.00
GLU107	H	1.00	0.000	1.00	0.00

**3.107.9 Detailed Probabilities of GLU107HG3:**

Overall probability: 1.000

Overall confidence: 0.857

**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLU107	1.00	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	0.000	1.00	0.00
GLU107	HB2	1.00	0.000	1.00	0.00
GLU107	HB3	1.00	0.000	1.00	0.00
GLU107	HG2	1.00	0.000	1.00	0.00
GLU107	HG3	1.00	0.000	1.00	0.00
GLU107	H	1.00	0.000	1.00	0.00

## 3.107.10 Detailed Probabilities of GLU107H:

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
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	0.000	1.00	0.00
GLU106	HB2	1.00	0.000	1.00	0.00
GLU106	HB3	1.00	0.000	1.00	0.00
GLU106	HG2	0.98	0.000	1.00	0.00
GLU106	HG3	0.97	0.000	1.00	0.00
GLU106	H	1.00	0.000	1.00	0.00
GLU107	HA	1.00	0.000	1.00	0.00
GLU107	HB2	1.00	0.005	1.00	0.00
GLU107	HB3	1.00	0.000	1.00	0.00
GLU107	HG2	1.00	0.000	1.00	0.00
GLU107	HG3	1.00	0.000	1.00	0.00
GLU107	H	1.00	0.000	1.00	0.00