

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.

2 Overall Reports

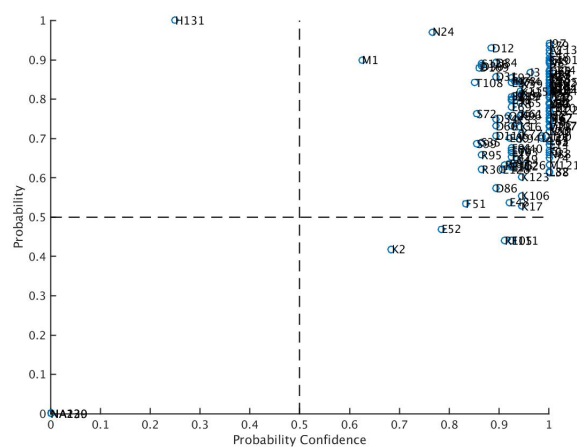
Figure: Overall 2D probabilities v.s. confidences2.1

Figures: Overall probabilities2.2

Figures: Probabilities of atoms for every residue2.3

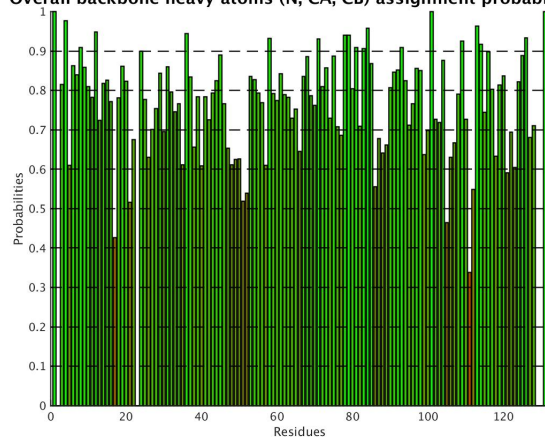
2.1 Overall 2D probabilities v.s. confidences

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

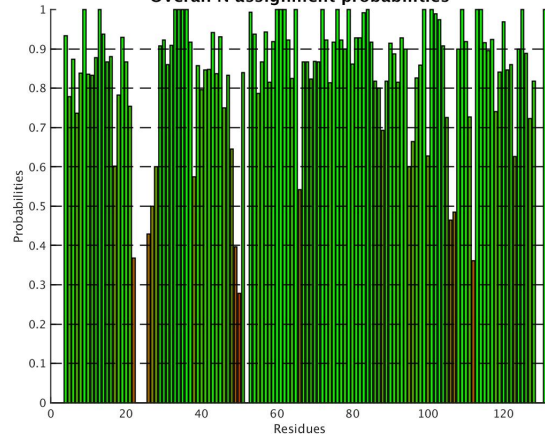


2.2 Figures: Overall Probabilities

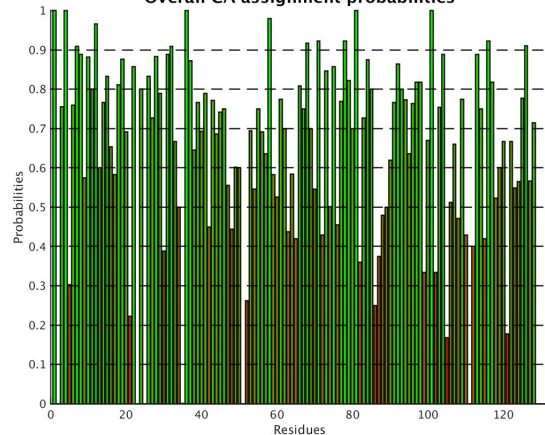
Overall backbone heavy atoms (N, CA, CB) assignment probabilities

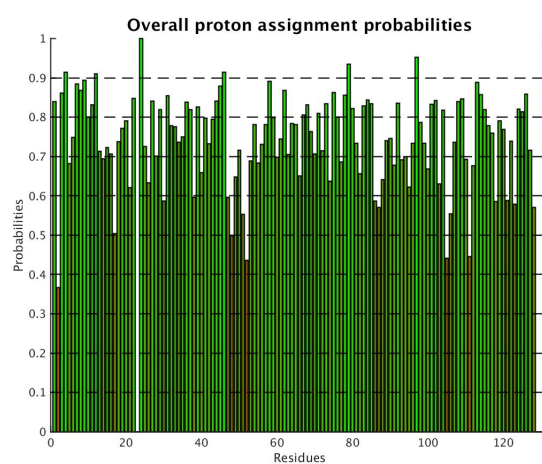


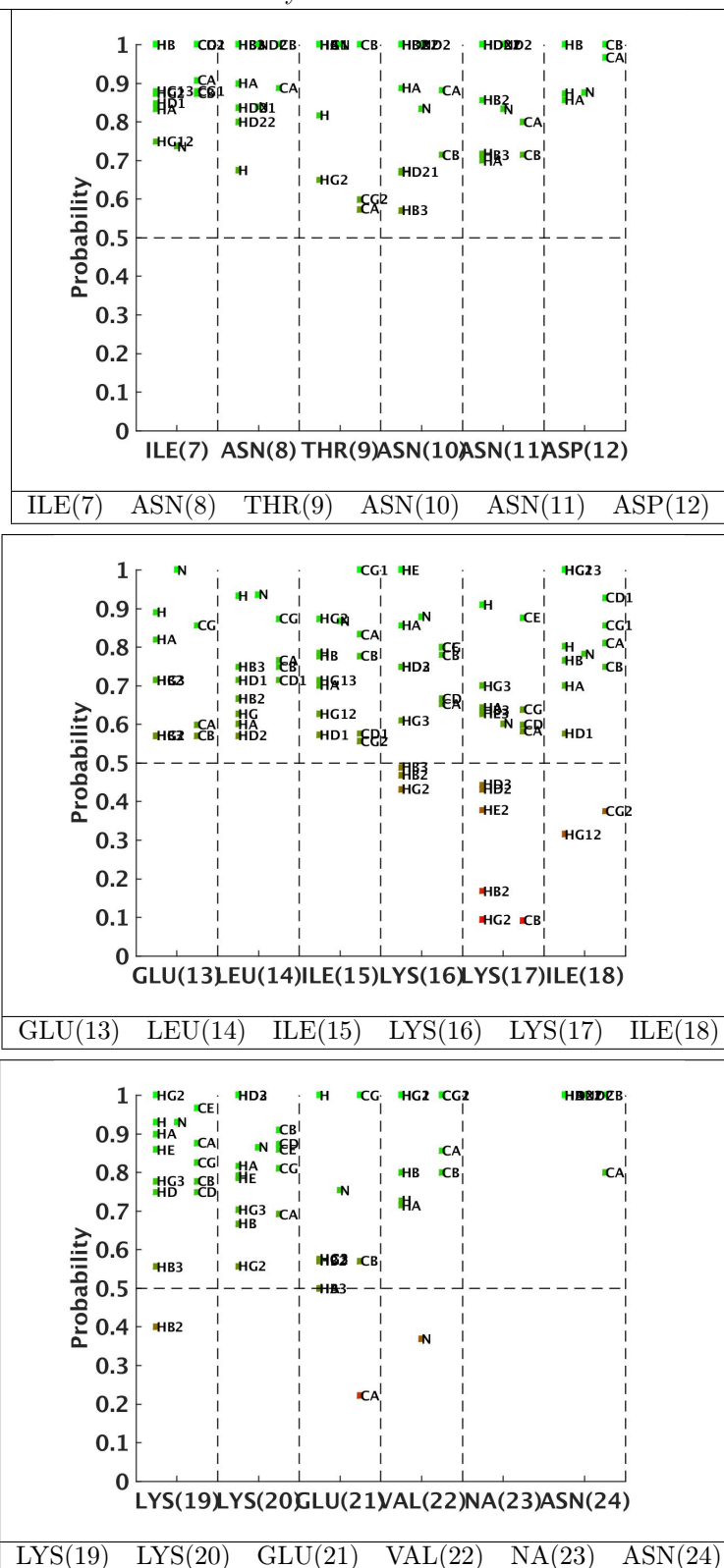
Overall N assignment probabilities

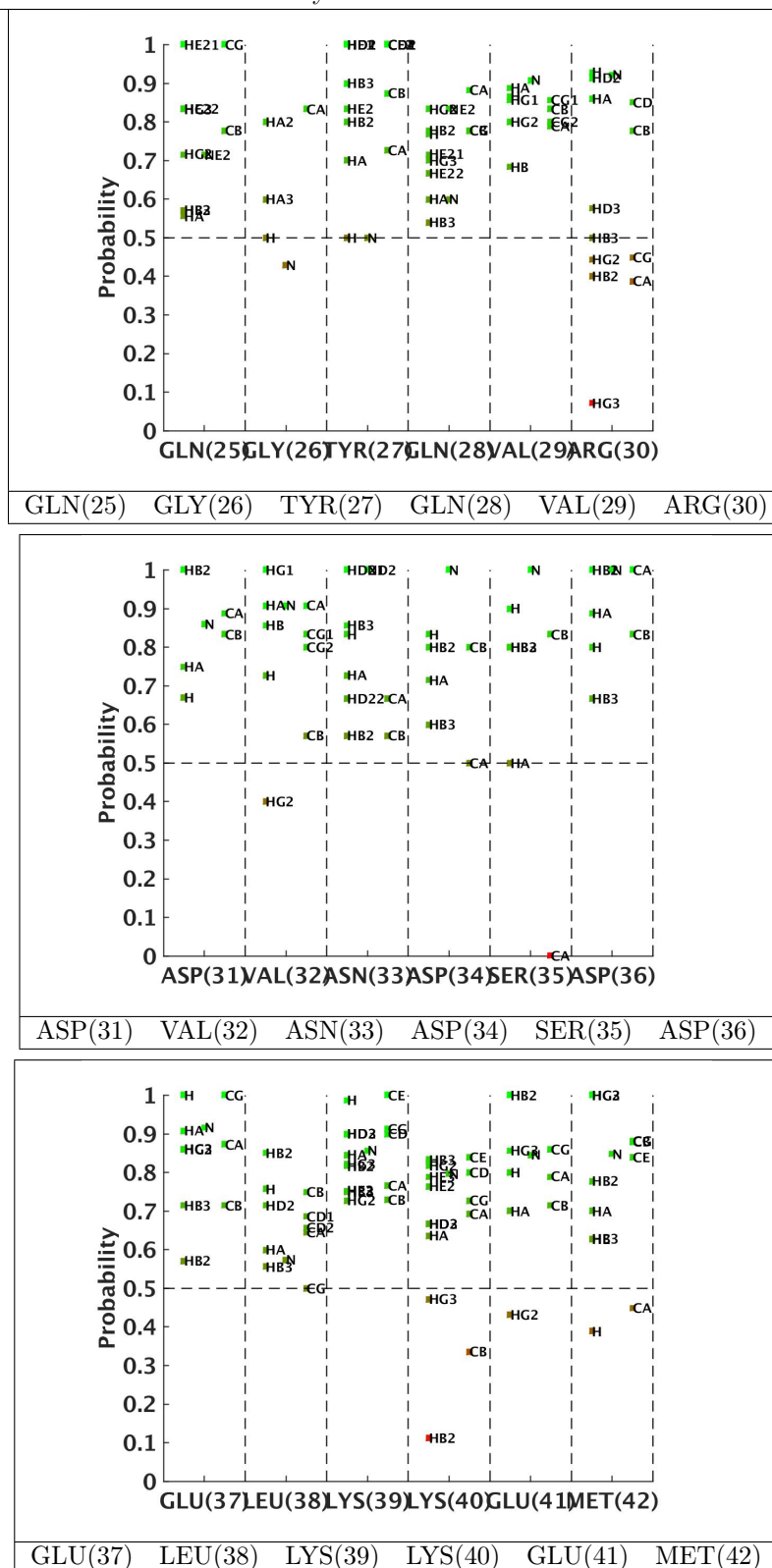


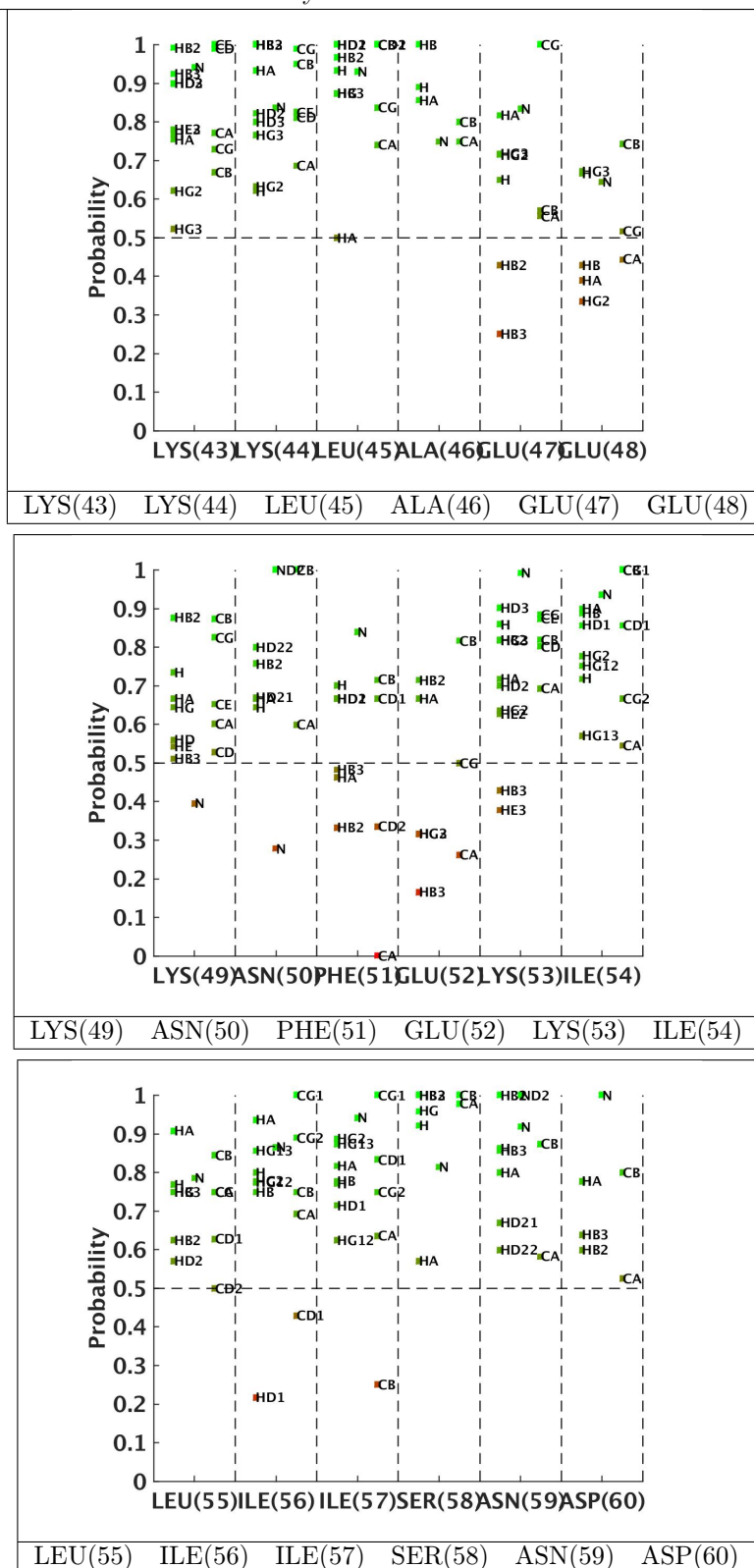
Overall CA assignment probabilities

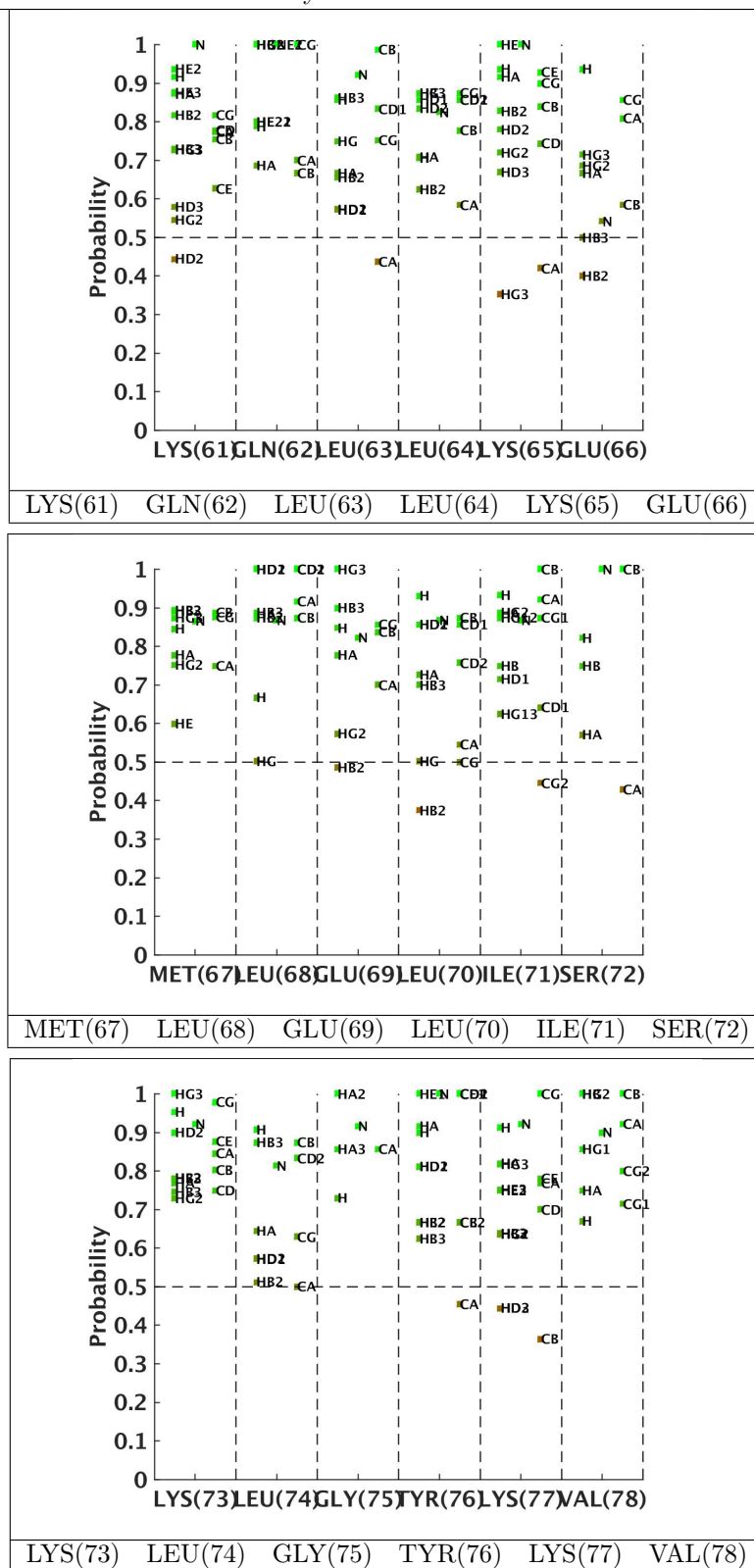


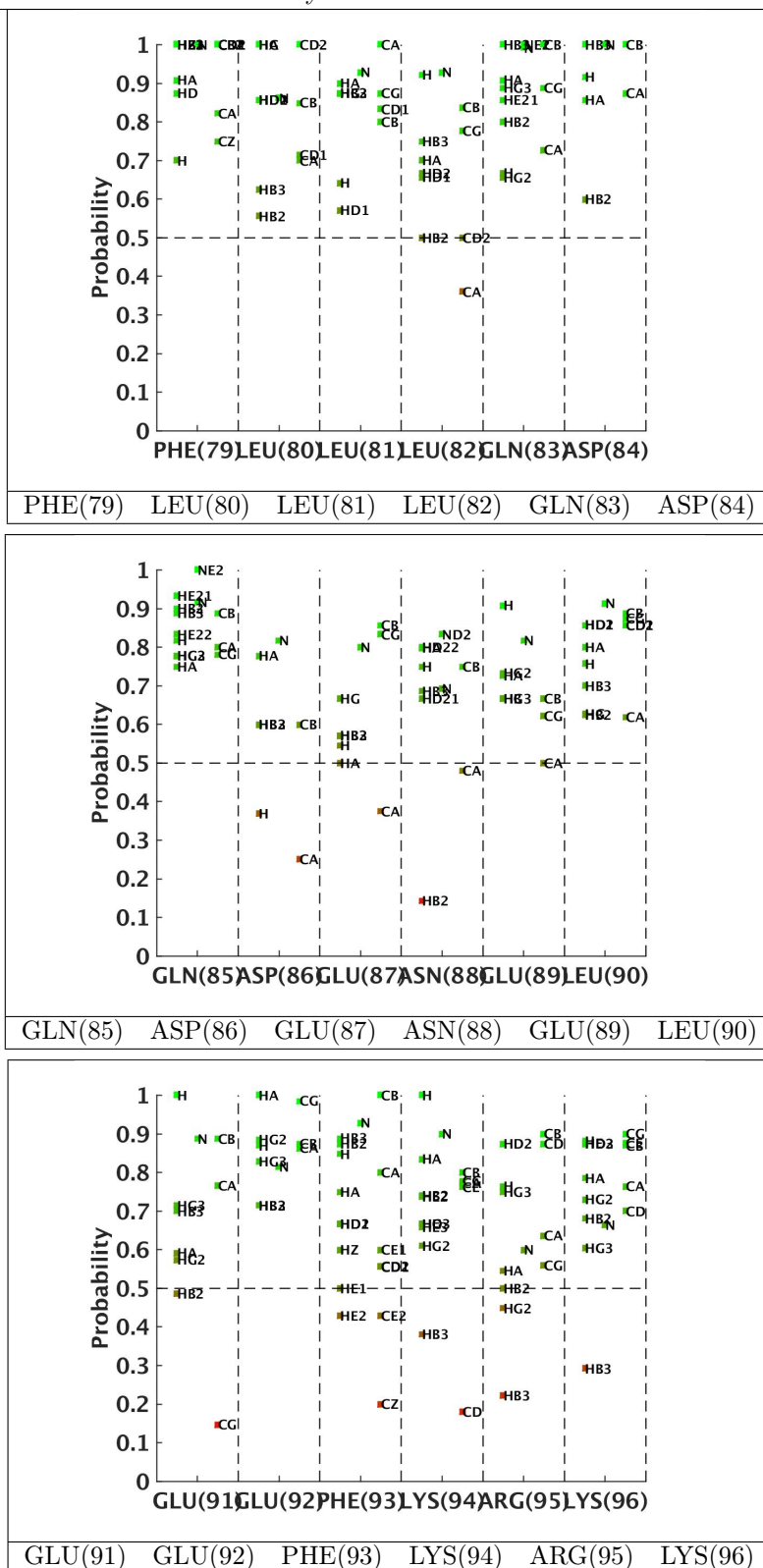
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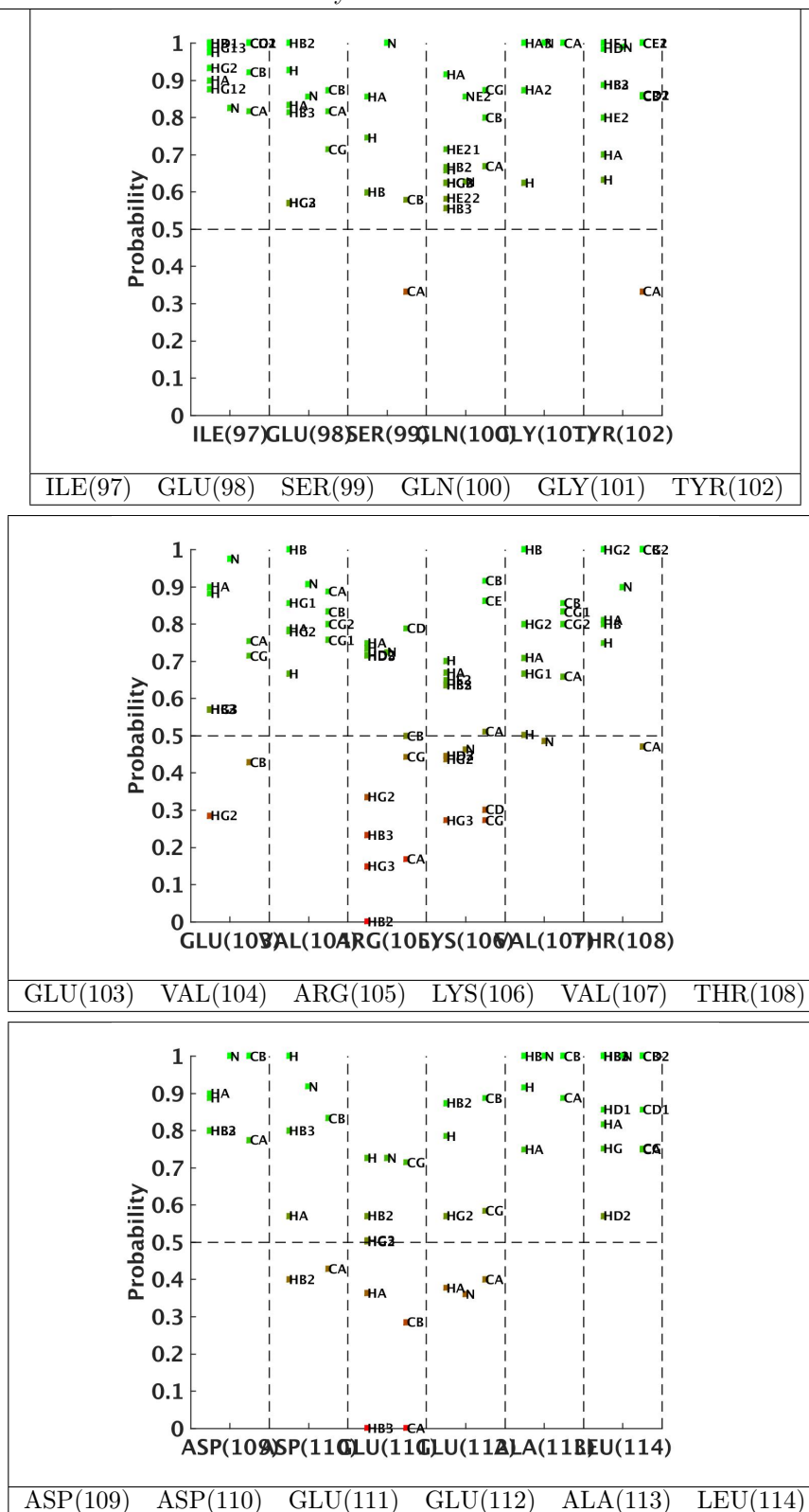


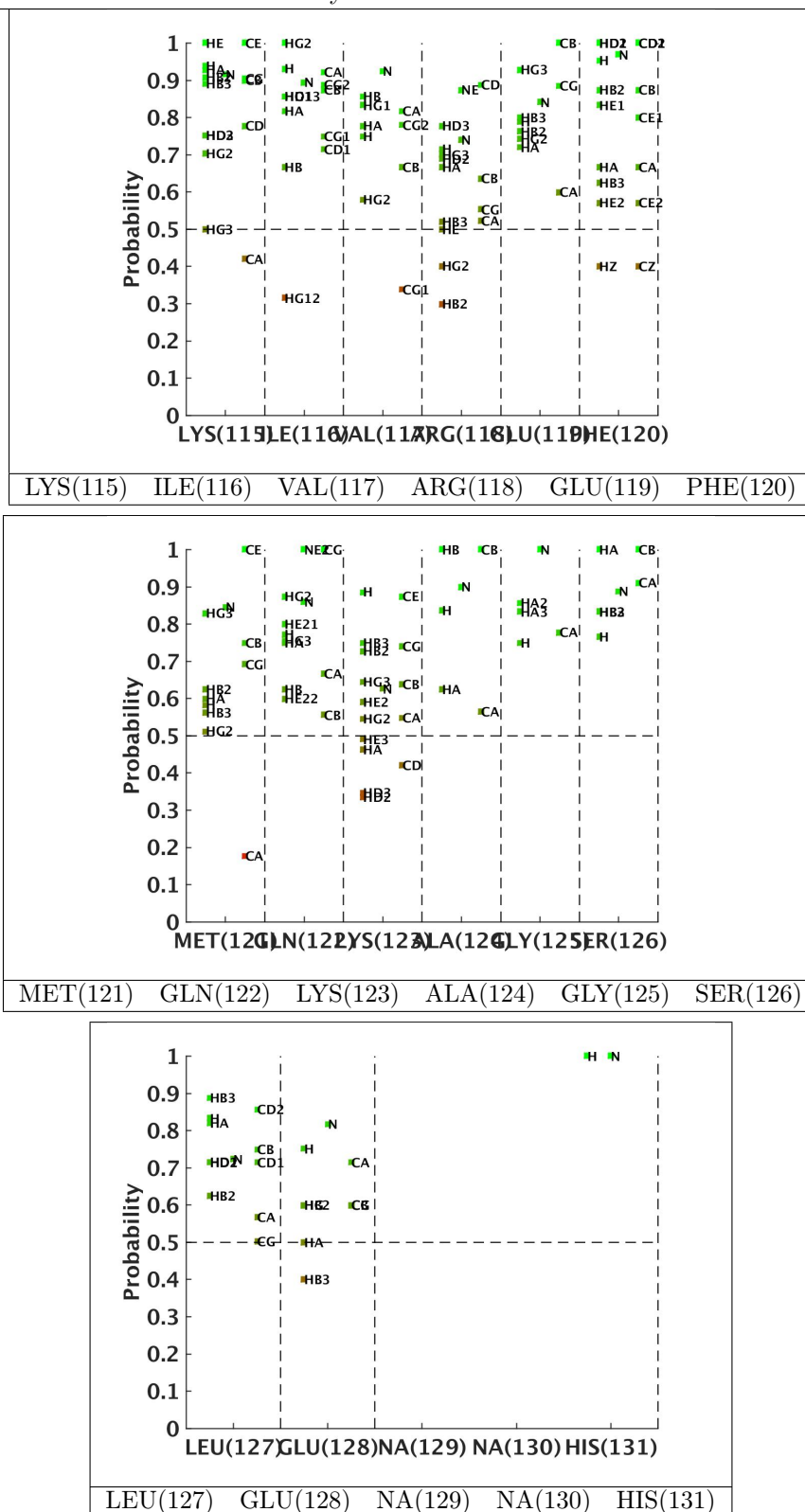












3 Residues Report

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.

MET(1)	LYS(2)	ILE(3)	LEU(4)	ILE(5)	LEU(6)
ILE(7)	ASN(8)	THR(9)	ASN(10)	ASN(11)	ASP(12)
GLU(13)	LEU(14)	ILE(15)	LYS(16)	LYS(17)	ILE(18)
LYS(19)	LYS(20)	GLU(21)	VAL(22)	NA(23)	ASN(24)
GLN(25)	GLY(26)	TYR(27)	GLN(28)	VAL(29)	ARG(30)
ASP(31)	VAL(32)	ASN(33)	ASP(34)	SER(35)	ASP(36)
GLU(37)	LEU(38)	LYS(39)	LYS(40)	GLU(41)	MET(42)
LYS(43)	LYS(44)	LEU(45)	ALA(46)	GLU(47)	GLU(48)
LYS(49)	ASN(50)	PHE(51)	GLU(52)	LYS(53)	ILE(54)
LEU(55)	ILE(56)	ILE(57)	SER(58)	ASN(59)	ASP(60)
LYS(61)	GLN(62)	LEU(63)	LEU(64)	LYS(65)	GLU(66)
MET(67)	LEU(68)	GLU(69)	LEU(70)	ILE(71)	SER(72)
LYS(73)	LEU(74)	GLY(75)	TYR(76)	LYS(77)	VAL(78)
PHE(79)	LEU(80)	LEU(81)	LEU(82)	GLN(83)	ASP(84)
GLN(85)	ASP(86)	GLU(87)	ASN(88)	GLU(89)	LEU(90)
GLU(91)	GLU(92)	PHE(93)	LYS(94)	ARG(95)	LYS(96)
ILE(97)	GLU(98)	SER(99)	GLN(100)	GLY(101)	TYR(102)
GLU(103)	VAL(104)	ARG(105)	LYS(106)	VAL(107)	THR(108)
ASP(109)	ASP(110)	GLU(111)	GLU(112)	ALA(113)	LEU(114)
LYS(115)	ILE(116)	VAL(117)	ARG(118)	GLU(119)	PHE(120)
MET(121)	GLN(122)	LYS(123)	ALA(124)	GLY(125)	SER(126)
LEU(127)	GLU(128)	NA(129)	NA(130)	HIS(131)	

3.1 MET(1)

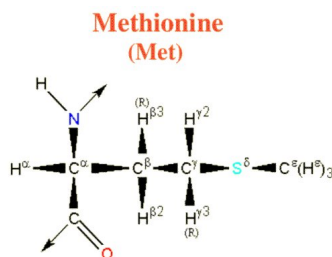


Figure 1: Image from the BMRB

Residue probability: 0.900

Residue probability confidence: 0.625

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	NA	—	—	0.000	0.000
CA 3.1.1	54.500	56.303	4.222	1.000	0.625
CB 3.1.2	33.173	33.217	4.564	1.000	0.625
CG 3.1.3	30.985	32.123	4.122	1.000	0.625
CE	NA	—	—	0.000	0.000
N	NA	—	—	0.000	0.000
HA 3.1.4	4.118	4.409	0.504	0.800	0.625
HB2 3.1.5	2.030	2.016	0.340	0.800	0.625
HB3 3.1.6	2.198	1.978	0.359	0.800	0.625
HG2 3.1.7	2.429	2.410	0.360	1.000	0.625
HG3 3.1.8	2.602	2.378	0.386	0.800	0.625
HE	NA	—	—	0.000	0.000
H	NA	—	—	0.000	0.000

3.1.1 Detailed Probabilities of MET1CA:

Overall probability: 1.000

Overall confidence: 0.625

Inter- and intra-residue probability

Residue	Probability	Confidence
MET1	1.00	0.83
LYS2	0.00	0.00

Expected NOESY Contacts

Proton	Expected probability
M1HB2	1.00
M1HB3	1.00
M1HG2	1.00
M1HG3	1.00
M1H	1.00
M1HA	1.00
K2H	1.00
K2HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET1	HA	1.00	0.026	1.00	9.26
MET1	HB2	1.00	0.003	1.00	0.24
MET1	HB3	1.00	0.004	1.00	0.44
MET1	HG2	1.00	0.002	1.00	0.21
MET1	HG3	1.00	0.008	1.00	0.12

3.1.2 Detailed Probabilities of MET1CB:

Overall probability: 1.000

Overall confidence: 0.625

Inter- and intra-residue probability

Residue	Probability	Confidence
MET1	1.00	0.71
LYS2	0.00	0.00

Expected NOESY Contacts

Proton	Expected probability
M1HA	1.00
M1HB2	1.00
M1HG2	1.00
M1HG3	1.00
M1HE1	0.97
M1H	1.00
M1HB3	1.00
K2H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET1	HA	1.00	0.001	1.00	0.35
MET1	HB2	1.00	0.008	1.00	4.04
MET1	HB3	1.00	0.006	1.00	7.09
MET1	HG2	1.00	0.020	1.00	1.43
MET1	HG3	1.00	0.008	1.00	0.47

3.1.3 Detailed Probabilities of MET1CG:

Overall probability: 1.000

Overall confidence: 0.625

Inter- and intra-residue probability

Residue	Probability	Confidence
MET1	1.00	0.71
LYS2	0.00	0.00

Expected NOESY Contacts

Proton	Expected probability
M1HA	1.00
M1HB2	1.00
M1HB3	1.00
M1HG2	1.00
M1HE1	1.00
M1H	1.00
M1HG3	1.00
K2H	0.95

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET1	HA	1.00	0.005	1.00	0.20
MET1	HB2	1.00	0.012	1.00	0.67
MET1	HB3	1.00	0.015	1.00	0.57
MET1	HG2	1.00	0.001	1.00	4.69
MET1	HG3	1.00	0.003	1.00	11.17

3.1.4 Detailed Probabilities of MET1HA:

Overall probability: 0.800

Overall confidence: 0.625

Inter- and intra-residue probability

Residue	Probability	Confidence
MET1	0.80	0.83
LYS2	0.00	0.00

Expected NOESY Contacts

Proton	Expected probability
M1HB2	1.00
M1HB3	1.00
M1HG2	1.00
M1HG3	1.00
M1H	1.00
M1HA	1.00
K2H	1.00
K2HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET1	HA	1.00	0.026	1.00	9.26
MET1	HB2	1.00	0.142	0.00	0.00
MET1	HB3	1.00	0.001	1.00	0.35
MET1	HG2	1.00	0.005	1.00	0.23
MET1	HG3	1.00	0.005	1.00	0.20

3.1.5 Detailed Probabilities of MET1HB2:

Overall probability: 0.800

Overall confidence: 0.625

Inter- and intra-residue probability

Residue	Probability	Confidence
MET1	0.80	0.71
LYS2	0.00	0.00

Expected NOESY Contacts

Proton	Expected probability
M1HA	1.00
M1HB3	1.00
M1HG2	1.00
M1HG3	1.00
M1HE1	0.96
M1H	1.00
M1HB2	1.00
K2H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET1	HA	1.00	0.003	1.00	0.24
MET1	HB2	1.00	0.006	1.00	7.54
MET1	HB3	1.00	0.008	1.00	4.04
MET1	HG2	1.00	0.126	0.00	0.00
MET1	HG3	1.00	0.012	1.00	0.67

3.1.6 Detailed Probabilities of MET1HB3:

Overall probability: 0.800

Overall confidence: 0.625

Inter- and intra-residue probability

Residue	Probability	Confidence
MET1	0.80	0.71
LYS2	0.00	0.00

Expected NOESY Contacts

Proton	Expected probability
M1HA	1.00
M1HB2	1.00
M1HG2	1.00
M1HG3	1.00
M1HE1	0.97
M1H	1.00
M1HB3	1.00
K2H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET1	HA	1.00	0.004	1.00	0.44
MET1	HB2	1.00	0.004	1.00	4.01
MET1	HB3	1.00	0.006	1.00	7.09
MET1	HG2	1.00	0.230	0.00	0.00
MET1	HG3	1.00	0.015	1.00	0.57

3.1.7 Detailed Probabilities of MET1HG2:

Overall probability: 1.000

Overall confidence: 0.625

Inter- and intra-residue probability

Residue	Probability	Confidence
MET1	1.00	0.71
LYS2	0.00	0.00

Expected NOESY Contacts

Proton	Expected probability
M1HA	1.00
M1HB2	1.00
M1HB3	1.00
M1HG3	1.00
M1HE1	1.00
M1H	1.00
M1HG2	1.00
K2H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET1	HA	1.00	0.002	1.00	0.21
MET1	HB2	1.00	0.021	1.00	1.05
MET1	HB3	1.00	0.020	1.00	1.43
MET1	HG2	1.00	0.001	1.00	10.63
MET1	HG3	1.00	0.001	1.00	4.69

3.1.8 Detailed Probabilities of MET1HG3:

Overall probability: 0.800

Overall confidence: 0.625

Inter- and intra-residue probability

Residue	Probability	Confidence
MET1	0.80	0.71
LYS2	0.00	0.00

Expected NOESY Contacts

Proton	Expected probability
M1HA	1.00
M1HB2	1.00
M1HB3	1.00
M1HG2	1.00
M1HE1	1.00
M1H	1.00
M1HG3	1.00
K2H	0.95

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET1	HA	1.00	0.008	1.00	0.12
MET1	HB2	1.00	0.004	1.00	0.43
MET1	HB3	1.00	0.008	1.00	0.47
MET1	HG2	1.00	0.174	0.00	0.00
MET1	HG3	1.00	0.003	1.00	11.17

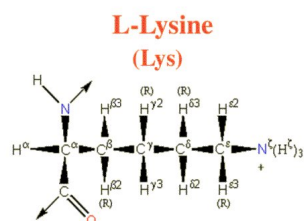


Figure 2: Image from the BMRB

Residue probability: 0.418
Residue probability confidence: 0.684

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	NA	—	—	0.000	0.000
CA	NA	—	—	0.000	0.000
CB	NA	—	—	0.000	0.000
CG 3.2.1	25.517	24.941	1.956	0.429	0.636
CD 3.2.2	28.798	29.020	2.193	0.633	0.667
CE 3.2.3	42.469	41.893	1.492	0.500	0.750
N	NA	—	—	0.000	0.000
NZ	NA	—	—	0.000	0.000
HA	NA	—	—	0.000	0.000
HB	NA	—	—	0.000	0.000
HG2 3.2.4	1.068	1.358	0.344	0.167	0.636
HG3 3.2.5	1.035	1.343	0.357	0.167	0.636
HD2 3.2.6	1.261	1.614	0.957	0.500	0.667
HD3 3.2.7	0.960	1.595	0.387	0.500	0.667
HE2 3.2.8	2.758	2.907	0.230	0.300	0.750
HE3 3.2.9	2.881	2.901	0.241	0.567	0.750
H	NA	—	—	0.000	0.000
HZ	NA	—	—	0.000	0.000

3.2.1 Detailed Probabilities of LYS2CG:

Overall probability: 0.429
Overall confidence: 0.636

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS2	0.33	0.60
ILE3	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K2HA	1.00
K2HB2	1.00
K2HG2	1.00
K2HD2	1.00
K2HD3	1.00
K2HE2	1.00
K2HE3	1.00
K2H	1.00
K2HZ2	1.00
K2HG3	1.00
I3H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS2	HG2	1.00	0.053	0.00	0.00
LYS2	HG3	1.00	0.020	1.00	54.17
LYS2	HD2	1.00	0.232	0.00	0.00
LYS2	HD3	1.00	0.055	0.00	0.00
LYS2	HE2	1.00	0.128	0.00	0.00
LYS2	HE3	1.00	0.005	1.00	0.09
ILE3	H	0.96	0.004	1.00	0.08

3.2.2 Detailed Probabilities of LYS2CD:

Overall probability: 0.633

Overall confidence: 0.667

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS2	0.63	0.67

Expected NOESY Contacts

Proton	Expected probability
K2HA	0.98
K2HB2	1.00
K2HG2	1.00
K2HG3	1.00
K2HD3	1.00
K2HE2	1.00
K2HE3	1.00
K2HZ2	1.00
K2HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS2	HG2	1.00	0.018	1.00	1.16
LYS2	HG3	1.00	0.051	0.00	0.00
LYS2	HD2	1.00	0.009	1.00	6.06
LYS2	HD3	1.00	0.002	1.00	1.39
LYS2	HE2	1.00	0.032	0.80	0.00
LYS2	HE3	1.00	0.155	0.00	0.00

3.2.3 Detailed Probabilities of LYS2CE:

Overall probability: 0.500

Overall confidence: 0.750

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS2	0.50	0.75

Expected NOESY Contacts

Proton	Expected probability
K2HB2	0.98
K2HG2	1.00
K2HG3	1.00
K2HD2	1.00
K2HD3	1.00
K2HE3	1.00
K2HZ2	1.00
K2HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS2	HG2	1.00	0.088	0.00	0.00
LYS2	HG3	1.00	0.055	0.00	0.00
LYS2	HD2	1.00	0.003	1.00	0.30
LYS2	HD3	1.00	0.020	1.00	0.38
LYS2	HE2	1.00	0.129	0.00	0.00
LYS2	HE3	1.00	0.006	1.00	2.15

3.2.4 Detailed Probabilities of LYS2HG2:

Overall probability: 0.167

Overall confidence: 0.636

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS2	0.17	0.60
ILE3	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K2HA	1.00
K2HB2	1.00
K2HG3	1.00
K2HD2	1.00
K2HD3	1.00
K2HE2	1.00
K2HE3	1.00
K2H	1.00
K2HZ2	1.00
K2HG2	1.00
I3H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS2	HG2	1.00	0.335	0.00	0.00
LYS2	HG3	1.00	0.053	0.00	0.00
LYS2	HD2	1.00	0.018	1.00	1.16
LYS2	HD3	1.00	0.194	0.00	0.00
LYS2	HE2	1.00	0.088	0.00	0.00
LYS2	HE3	1.00	0.095	0.00	0.00

3.2.5 Detailed Probabilities of LYS2HG3:

Overall probability: 0.167

Overall confidence: 0.636

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS2	0.17	0.60
ILE3	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K2HA	1.00
K2HB2	1.00
K2HG2	1.00
K2HD2	1.00
K2HD3	1.00
K2HE2	1.00
K2HE3	1.00
K2H	1.00
K2HZ2	1.00
K2HG3	1.00
I3H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS2	HG2	1.00	0.302	0.00	0.00
LYS2	HG3	1.00	0.020	1.00	54.17
LYS2	HD2	1.00	0.051	0.00	0.00
LYS2	HD3	1.00	0.227	0.00	0.00
LYS2	HE2	1.00	0.055	0.00	0.00
LYS2	HE3	1.00	0.062	0.00	0.00

3.2.6 Detailed Probabilities of LYS2HD2:

Overall probability: 0.500

Overall confidence: 0.667

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS2	0.50	0.67

Expected NOESY Contacts

Proton	Expected probability
K2HA	0.98
K2HB2	1.00
K2HG2	1.00
K2HG3	1.00
K2HD3	1.00
K2HE2	1.00
K2HE3	1.00
K2HZ2	1.00
K2HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS2	HG2	1.00	0.528	0.00	0.00
LYS2	HG3	1.00	0.232	0.00	0.00
LYS2	HD2	1.00	0.009	1.00	6.06
LYS2	HD3	1.00	0.001	1.00	0.83
LYS2	HE2	1.00	0.003	1.00	0.30
LYS2	HE3	1.00	0.288	0.00	0.00

3.2.7 Detailed Probabilities of LYS2HD3:

Overall probability: 0.500

Overall confidence: 0.667

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS2	0.50	0.67

Expected NOESY Contacts

Proton	Expected probability
K2HA	0.98
K2HB2	1.00
K2HG2	1.00
K2HG3	1.00
K2HD2	1.00
K2HE2	1.00
K2HE3	1.00
K2HZ2	1.00
K2HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS2	HG2	1.00	0.227	0.00	0.00
LYS2	HG3	1.00	0.055	0.00	0.00
LYS2	HD2	1.00	0.002	1.00	1.39
LYS2	HD3	1.00	0.162	0.00	0.00
LYS2	HE2	1.00	0.020	1.00	0.38
LYS2	HE3	1.00	0.013	1.00	0.28

3.2.8 Detailed Probabilities of LYS2HE2:

Overall probability: 0.300

Overall confidence: 0.750

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS2	0.30	0.75

Expected NOESY Contacts

Proton	Expected probability
K2HB2	0.98
K2HG2	1.00
K2HG3	1.00
K2HD2	1.00
K2HD3	1.00
K2HE3	1.00
K2HZ2	1.00
K2HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS2	HG2	1.00	0.011	1.00	0.10
LYS2	HG3	1.00	0.128	0.00	0.00
LYS2	HD2	1.00	0.032	0.80	0.00
LYS2	HD3	1.00	0.652	0.00	0.00
LYS2	HE2	1.00	0.129	0.00	0.00
LYS2	HE3	1.00	0.485	0.00	0.00

3.2.9 Detailed Probabilities of LYS2HE3:

Overall probability: 0.567

Overall confidence: 0.750

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS2	0.57	0.75

Expected NOESY Contacts

Proton	Expected probability
K2HB2	0.99
K2HG2	1.00
K2HG3	1.00
K2HD2	1.00
K2HD3	1.00
K2HE2	1.00
K2HZ2	1.00
K2HE3	1.00

NOESY contacts detailed probability					
Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS2	HG2	1.00	0.002	1.00	0.08
LYS2	HG3	1.00	0.005	1.00	0.09
LYS2	HD2	1.00	0.155	0.00	0.00
LYS2	HD3	1.00	0.579	0.00	0.00
LYS2	HE2	1.00	0.006	1.00	2.15
LYS2	HE3	1.00	0.036	0.40	0.00

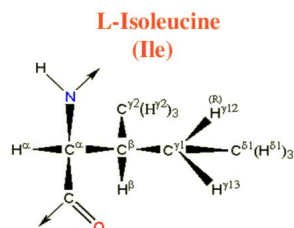


Figure 3: Image from the BMRB

Residue probability: 0.869
 Residue probability confidence: 0.963

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	173.405	175.926	2.710	0.000	0.000
CA 3.3.1	59.556	61.717	4.152	0.756	0.900
CB 3.3.2	40.508	38.702	3.945	0.875	1.000
CG1 3.3.3	27.378	27.785	2.037	0.875	1.000
CG2 3.3.4	17.852	17.574	1.928	0.889	1.000
CD1 3.3.5	13.477	13.545	3.646	1.000	1.000
N	NA	—	—	0.000	0.000
HA 3.3.6	4.826	4.185	1.403	1.000	0.900
HB 3.3.7	1.806	1.776	0.310	0.875	1.000
HG12 3.3.8	1.561	1.271	0.411	0.543	1.000
HG13 3.3.9	1.222	1.186	0.426	1.000	1.000
HG2 3.3.10	1.077	0.762	0.283	1.000	1.000
HD1 3.3.11	0.969	0.668	0.293	0.833	1.000
H 3.3.12	8.444	8.301	0.685	0.781	0.750

3.3.1 Detailed Probabilities of ILE3CA:

Overall probability: 0.756
 Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS2	0.00	0.00
ILE3	0.83	1.00
LEU4	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K2HA	1.00
I3HB	1.00
I3HG12	1.00
I3HG13	1.00
I3HG21	1.00
I3HD11	0.97
I3H	1.00
I3HA	1.00
L4H	1.00
L4HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE3	HA	1.00	0.003	1.00	0.70
ILE3	HB	1.00	0.058	0.00	0.00
ILE3	HG12	1.00	0.032	0.80	0.00
ILE3	HG13	1.00	0.019	1.00	1.01
ILE3	HG21	1.00	0.014	1.00	0.21
ILE3	HD11	0.97	0.013	1.00	0.29
ILE3	H	1.00	0.017	1.00	0.28
LEU4	HA	1.00	0.006	1.00	0.15
LEU4	H	1.00	0.095	0.00	0.00

3.3.2 Detailed Probabilities of ILE3CB:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE3	0.86	1.00
LEU4	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I3HA	1.00
I3HG12	1.00
I3HG13	1.00
I3HG21	1.00
I3HD11	1.00
I3H	1.00
I3HB	1.00
L4H	1.00

NOESY contacts detailed probability

3.3 ILE(3)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE3	HA	1.00	0.004	1.00	0.17
ILE3	HB	1.00	0.010	1.00	3.00
ILE3	HG12	1.00	0.054	0.00	0.00
ILE3	HG13	1.00	0.007	1.00	0.33
ILE3	HG21	1.00	0.002	1.00	0.87
ILE3	HD11	1.00	0.005	1.00	0.52
ILE3	H	1.00	0.000	1.00	0.21
LEU4	H	1.00	0.004	1.00	0.08

3.3.3 Detailed Probabilities of ILE3CG1:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE3	0.86	1.00
LEU4	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I3HA	1.00
I3HB	1.00
I3HG13	1.00
I3HG21	1.00
I3HD11	1.00
I3H	1.00
I3HG12	1.00
L4H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE3	HA	1.00	0.012	1.00	0.18
ILE3	HB	1.00	0.015	1.00	1.10
ILE3	HG12	1.00	0.223	0.00	0.00
ILE3	HG13	1.00	0.003	1.00	2.02
ILE3	HG21	1.00	0.018	1.00	1.02
ILE3	HD11	1.00	0.002	1.00	1.06
ILE3	H	1.00	0.005	1.00	0.10
LEU4	H	0.98	0.022	1.00	0.11

3.3.4 Detailed Probabilities of ILE3CG2:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE3	0.86	1.00
LEU4	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I3HA	1.00
I3HB	1.00
I3HG12	1.00
I3HG13	1.00
I3HG22	1.00
I3HD11	0.99
I3H	1.00
L4H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE3	HA	1.00	0.009	1.00	0.72
ILE3	HB	1.00	0.007	1.00	1.51
ILE3	HG12	1.00	0.045	0.00	0.00
ILE3	HG13	1.00	0.002	1.00	0.81
ILE3	HG21	1.00	0.002	1.00	29.49
ILE3	HD11	0.99	0.007	1.00	1.55
ILE3	H	1.00	0.009	1.00	0.15
LEU4	H	0.98	0.004	1.00	0.63
LEU4	HA	0.69	0.001	1.00	0.10

3.3.5 Detailed Probabilities of ILE3CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE3	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I3HA	0.97
I3HB	1.00
I3HG12	1.00
I3HG13	1.00
I3HG21	0.99
I3HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE3	HA	0.97	0.005	1.00	0.48
ILE3	HB	1.00	0.021	1.00	1.20
ILE3	HG12	1.00	0.027	1.00	1.64
ILE3	HG13	1.00	0.000	1.00	1.47
ILE3	HG21	0.99	0.014	1.00	1.60
ILE3	HD11	1.00	0.003	1.00	50.18
ILE3	H	0.94	0.008	1.00	0.10

3.3.6 Detailed Probabilities of ILE3HA:

Overall probability: 1.000

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS2	0.00	0.00
ILE3	1.00	1.00
LEU4	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K2HA	1.00
I3HB	1.00
I3HG12	1.00
I3HG13	1.00
I3HG21	1.00
I3HD11	0.97
I3H	1.00
I3HA	1.00
L4H	1.00
L4HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE3	HA	1.00	0.003	1.00	0.70
ILE3	HB	1.00	0.004	1.00	0.17
ILE3	HG12	1.00	0.012	1.00	0.18
ILE3	HG13	1.00	0.009	1.00	0.19
ILE3	HG21	1.00	0.009	1.00	0.72
ILE3	HD11	0.97	0.005	1.00	0.48
LEU4	HA	1.00	0.014	1.00	0.06
LEU4	H	1.00	0.009	1.00	-1542108.00

3.3.7 Detailed Probabilities of ILE3HB:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE3	0.83	1.00
LEU4	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I3HA	1.00
I3HG12	1.00
I3HG13	1.00
I3HG21	1.00
I3HD11	1.00
I3H	1.00
I3HB	1.00
L4H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE3	HA	1.00	0.058	0.00	0.00
ILE3	HB	1.00	0.010	1.00	3.00
ILE3	HG12	1.00	0.015	1.00	1.10
ILE3	HG13	1.00	0.019	1.00	0.47
ILE3	HG21	1.00	0.007	1.00	1.51
ILE3	HD11	1.00	0.021	1.00	1.20
LEU4	H	1.00	0.020	1.00	-249856.00
LEU4	HA	0.89	0.012	1.00	0.06

3.3.8 Detailed Probabilities of ILE3HG12:

Overall probability: 0.543

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE3	0.47	1.00
LEU4	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I3HA	1.00
I3HB	1.00
I3HG13	1.00
I3HG21	1.00
I3HD11	1.00
I3H	1.00
I3HG12	1.00
L4H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE3	HA	1.00	0.032	0.80	0.00
ILE3	HB	1.00	0.054	0.00	0.00
ILE3	HG12	1.00	0.223	0.00	0.00
ILE3	HG13	1.00	0.003	1.00	1.73
ILE3	HG21	1.00	0.045	0.00	0.00
ILE3	HD11	1.00	0.027	1.00	1.64
LEU4	H	0.98	0.016	1.00	-212969.00

3.3.9 Detailed Probabilities of ILE3HG13:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE3	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I3HA	1.00
I3HB	1.00
I3HG12	1.00
I3HG21	1.00
I3HD11	1.00
I3H	1.00
I3HG13	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE3	HA	1.00	0.019	1.00	1.01
ILE3	HB	1.00	0.007	1.00	0.33
ILE3	HG12	1.00	0.003	1.00	2.02
ILE3	HG13	1.00	0.028	1.00	5.04
ILE3	HG21	1.00	0.002	1.00	0.81
ILE3	HD11	1.00	0.000	1.00	1.47

3.3.10 Detailed Probabilities of ILE3HG21:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE3	1.00	1.00
LEU4	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I3HA	1.00
I3HB	1.00
I3HG12	1.00
I3HG13	1.00
I3HG22	1.00
I3HD11	0.99
I3H	1.00
L4H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE3	HA	1.00	0.014	1.00	0.21
ILE3	HB	1.00	0.002	1.00	0.87
ILE3	HG12	1.00	0.018	1.00	1.02
ILE3	HG13	1.00	0.006	1.00	0.49
ILE3	HG21	1.00	0.002	1.00	29.49
ILE3	HD11	0.99	0.014	1.00	1.60
LEU4	H	0.98	0.002	1.00	-597330.00
LEU4	HA	0.69	0.005	1.00	0.09

3.3.11 Detailed Probabilities of ILE3HD11:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE3	0.83	1.00

Expected NOESY Contacts

Proton	Expected probability
I3HA	0.97
I3HB	1.00
I3HG12	1.00
I3HG13	1.00
I3HG21	0.99
I3HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE3	HA	0.97	0.013	1.00	0.29
ILE3	HB	1.00	0.005	1.00	0.52
ILE3	HG12	1.00	0.002	1.00	1.06
ILE3	HG13	1.00	0.114	0.00	0.00
ILE3	HG21	0.99	0.007	1.00	1.55
ILE3	HD11	1.00	0.003	1.00	50.18

3.3.12 Detailed Probabilities of ILE3H:

Overall probability: 0.781

Overall confidence: 0.750

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS2	0.52	0.40
ILE3	1.00	1.00
LEU4	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K2H	1.00
K2HG2	0.97
K2HG3	0.96
K2HA	1.00
K2HB2	1.00
I3HA	1.00
I3HB	1.00
I3HG12	1.00
I3HG13	1.00
I3HG21	1.00
I3H	1.00
L4H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS2	HG2	0.97	1.588	0.03	0.00
LYS2	HG3	0.96	0.004	1.00	0.08
ILE3	HA	1.00	0.017	1.00	0.28
ILE3	HB	1.00	0.000	1.00	0.21
ILE3	HG12	1.00	0.005	1.00	0.10
ILE3	HG13	1.00	0.004	1.00	0.08
ILE3	HG21	1.00	0.009	1.00	0.15
ILE3	HD11	0.94	0.008	1.00	0.10
LEU4	H	1.00	0.060	0.00	0.00

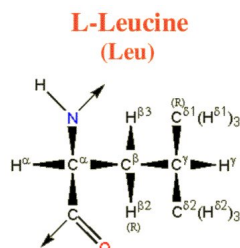
3.4 LEU(4)

Figure 4: Image from the BMRB

Residue probability: 0.917

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.832	177.056	1.929	0.000	0.000
CA 3.4.1	53.341	55.735	3.802	1.000	1.000
CB 3.4.2	45.313	42.389	3.750	1.000	1.000
CG 3.4.3	28.192	26.892	3.086	0.586	1.000
CD1 3.4.4	25.457	24.837	3.657	1.000	1.000
CD2 3.4.5	25.983	24.201	3.117	1.000	1.000
N 3.4.6	127.785	121.785	4.943	0.933	1.000
HA 3.4.7	5.459	4.315	0.840	0.900	1.000
HB 3.4.8	1.437	1.601	0.373	1.000	1.000
HG 3.4.9	1.451	1.510	0.340	1.000	1.000
HD1 3.4.10	0.642	0.739	0.294	0.833	1.000
HD2 3.4.11	0.678	0.727	0.421	0.833	1.000
H 3.4.12	9.081	8.237	0.647	0.917	1.000

3.4.1 Detailed Probabilities of LEU4CA:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE3	1.00	1.00
LEU4	1.00	1.00
ILE5	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I3HA	1.00
L4HB2	1.00
L4HG	1.00
L4HD11	0.99
L4HD21	0.99
L4H	1.00
L4HA	1.00
I5H	1.00
I5HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE3	HA	1.00	0.014	1.00	0.06
ILE3	HB	0.89	0.012	1.00	0.06
ILE3	HG21	0.71	0.005	1.00	0.09
LEU4	HA	1.00	0.000	1.00	1.52
LEU4	HB2	1.00	0.005	1.00	0.48
LEU4	HG	1.00	0.009	1.00	0.48
LEU4	HD11	0.99	0.011	1.00	0.39
LEU4	HD21	0.99	0.025	1.00	0.39
LEU4	H	1.00	0.001	1.00	0.10
ILE5	HA	1.00	0.007	1.00	0.06
ILE5	H	1.00	0.005	1.00	0.61

3.4.2 Detailed Probabilities of LEU4CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU4	1.00	1.00
ILE5	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L4HA	1.00
L4HB3	1.00
L4HG	1.00
L4HD11	1.00
L4HD21	1.00
L4H	1.00
I5H	1.00

NOESY contacts detailed probability

3.4 LEU(4)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU4	HA	1.00	0.001	1.00	0.41
LEU4	HB2	1.00	0.005	1.00	5.37
LEU4	HG	1.00	0.009	1.00	5.37
LEU4	HD11	1.00	0.019	1.00	1.37
LEU4	HD21	1.00	0.017	1.00	1.37
LEU4	H	1.00	0.002	1.00	0.39
ILE5	H	1.00	0.014	1.00	0.11
ILE5	HA	0.92	0.011	1.00	0.12

3.4.3 Detailed Probabilities of LEU4CG:

Overall probability: 0.586

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU4	0.67	1.00
ILE5	0.10	1.00

Expected NOESY Contacts

Proton	Expected probability
L4HA	1.00
L4HB2	1.00
L4HD11	1.00
L4HD21	1.00
L4H	1.00
L4HG	1.00
I5H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU4	HA	1.00	0.002	1.00	0.25
LEU4	HB2	1.00	0.022	1.00	12.32
LEU4	HG	1.00	0.008	1.00	12.32
LEU4	HD11	1.00	0.078	0.00	0.00
LEU4	HD21	1.00	0.042	0.00	0.00
LEU4	H	1.00	0.001	1.00	0.21
ILE5	H	0.99	0.039	0.10	0.00

3.4.4 Detailed Probabilities of LEU4CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU4	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L4HA	0.99
L4HB2	1.00
L4HG	1.00
L4HD12	1.00
L4HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU4	HA	0.99	0.002	1.00	0.52
LEU4	HB2	1.00	0.006	1.00	3.17
LEU4	HG	1.00	0.008	1.00	3.17
LEU4	HD11	1.00	0.006	1.00	74.03
LEU4	HD21	1.00	0.030	1.00	0.00
LEU4	H	0.86	0.006	1.00	0.29

3.4.5 Detailed Probabilities of LEU4CD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU4	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L4HA	0.99
L4HB2	1.00
L4HG	1.00
L4HD11	1.00
L4HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU4	HA	0.99	0.002	1.00	0.52
LEU4	HB2	1.00	0.006	1.00	3.17
LEU4	HG	1.00	0.008	1.00	3.17
LEU4	HD11	1.00	0.006	1.00	74.03
LEU4	HD21	1.00	0.030	1.00	0.00
LEU4	H	0.85	0.006	1.00	0.29

3.4.6 Detailed Probabilities of LEU4N:

Overall probability: 0.933

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE3	0.83	1.00
LEU4	1.00	1.00
ILE5	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I3HG21	0.98
I3HG12	0.98
I3HA	1.00
I3HB	1.00
I3H	1.00
L4HA	1.00
L4HB2	1.00
L4HG	1.00
L4H	1.00
I5H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE3	HA	1.00	0.009	1.00	-1542108.00
ILE3	HB	1.00	0.020	1.00	-249856.00
ILE3	HG12	0.98	0.016	1.00	-212969.00
ILE3	HG21	0.98	0.002	1.00	-597330.00
ILE3	H	1.00	0.060	0.00	0.00
ILE3	HG13	0.93	0.018	1.00	-91843.00
LEU4	HA	1.00	0.003	1.00	-266303.00
LEU4	HB2	1.00	0.004	1.00	-940305.00
LEU4	HG	1.00	0.010	1.00	-940305.00
LEU4	H	1.00	0.001	1.00	-4247564.00
LEU4	HD11	0.88	0.013	1.00	-421823.00
LEU4	HD21	0.87	0.023	1.00	-421823.00
ILE5	H	1.00	0.019	1.00	-121633.00
ILE5	HA	0.93	0.002	1.00	-1542108.00
ILE5	HG13	0.58	0.018	1.00	-134908.00

3.4.7 Detailed Probabilities of LEU4HA:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE3	1.00	1.00
LEU4	1.00	1.00
ILE5	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
I3HA	1.00
L4HB2	1.00
L4HG	1.00
L4HD11	0.99
L4HD21	0.99
L4H	1.00
L4HA	1.00
I5H	1.00
I5HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE3	HA	1.00	0.006	1.00	0.15
ILE3	HG21	0.71	0.001	1.00	0.10
LEU4	HA	1.00	0.000	1.00	1.52
LEU4	HB2	1.00	0.001	1.00	0.41
LEU4	HG	1.00	0.002	1.00	0.25
LEU4	HD11	0.99	0.002	1.00	0.52
LEU4	HD21	0.99	0.002	1.00	0.52
LEU4	H	1.00	0.003	1.00	-266303.00
ILE5	HA	1.00	0.189	0.00	0.00
ILE5	H	1.00	0.000	1.00	-702003.00

3.4.8 Detailed Probabilities of LEU4HB2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU4	1.00	1.00
ILE5	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L4HA	1.00
L4HB3	1.00
L4HG	1.00
L4HD11	1.00
L4HD21	1.00
L4H	1.00
I5H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU4	HA	1.00	0.005	1.00	0.48
LEU4	HB2	1.00	0.005	1.00	5.37
LEU4	HG	1.00	0.022	1.00	12.32
LEU4	HD11	1.00	0.006	1.00	3.17
LEU4	HD21	1.00	0.006	1.00	3.17
LEU4	H	1.00	0.004	1.00	-940305.00
ILE5	H	1.00	0.004	1.00	-259686.00

3.4.9 Detailed Probabilities of LEU4HG:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU4	1.00	1.00
ILE5	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L4HA	1.00
L4HB2	1.00
L4HD11	1.00
L4HD21	1.00
L4H	1.00
L4HG	1.00
I5H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU4	HA	1.00	0.009	1.00	0.48
LEU4	HB2	1.00	0.009	1.00	5.37
LEU4	HG	1.00	0.008	1.00	12.32
LEU4	HD11	1.00	0.008	1.00	3.17
LEU4	HD21	1.00	0.008	1.00	3.17
LEU4	H	1.00	0.010	1.00	-940305.00
ILE5	H	0.99	0.010	1.00	-259686.00

3.4.10 Detailed Probabilities of LEU4HD11:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU4	0.83	1.00

Expected NOESY Contacts

Proton	Expected probability
L4HA	0.99
L4HB2	1.00
L4HG	1.00
L4HD12	1.00
L4HD21	1.00

NOESY contacts detailed probability

3.4 LEU(4)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU4	HA	0.99	0.011	1.00	0.39
LEU4	HB2	1.00	0.019	1.00	1.37
LEU4	HG	1.00	0.078	0.00	0.00
LEU4	HD11	1.00	0.006	1.00	74.03
LEU4	HD21	1.00	0.006	1.00	74.03
LEU4	H	0.86	0.013	1.00	-421823.00

3.4.11 Detailed Probabilities of LEU4HD21:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU4	0.83	1.00

Expected NOESY Contacts

Proton	Expected probability
L4HA	0.99
L4HB2	1.00
L4HG	1.00
L4HD11	1.00
L4HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU4	HA	0.99	0.025	1.00	0.39
LEU4	HB2	1.00	0.017	1.00	1.37
LEU4	HG	1.00	0.042	0.00	0.00
LEU4	HD11	1.00	0.030	1.00	0.00
LEU4	HD21	1.00	0.030	1.00	0.00
LEU4	H	0.85	0.023	1.00	-421823.00

3.4.12 Detailed Probabilities of LEU4H:

Overall probability: 0.917

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE3	0.80	1.00
LEU4	1.00	1.00
ILE5	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I3HG21	0.98
I3HG12	0.98
I3HA	1.00
I3HB	1.00
I3H	1.00
L4HA	1.00
L4HB2	1.00
L4HG	1.00
L4H	1.00
I5H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE3	HA	1.00	0.095	0.00	0.00
ILE3	HB	1.00	0.004	1.00	0.08
ILE3	HG12	0.98	0.022	1.00	0.11
ILE3	HG21	0.98	0.004	1.00	0.63
ILE3	HG13	0.93	0.001	1.00	0.13
LEU4	HA	1.00	0.001	1.00	0.10
LEU4	HB2	1.00	0.002	1.00	0.39
LEU4	HG	1.00	0.001	1.00	0.21
LEU4	H	1.00	0.001	1.00	-4247564.00
LEU4	HD11	0.88	0.006	1.00	0.29
LEU4	HD21	0.87	0.006	1.00	0.29
ILE5	H	1.00	0.011	1.00	-79576.00

L-Isoleucine (Ile)

The diagram shows the chemical structure of L-Isoleucine. It features a central chiral carbon atom (C^α) bonded to a hydrogen atom (H^{α2}), an amino group (NH²), a carboxyl group (COOH), and a side chain. The side chain consists of a methylene group (C^β) bonded to a CH group (C^{γ1}). This CH group is further substituted with a hydrogen atom (H^{γ12}) and a methyl group (CH₃, labeled H^{γ13}). The C^{γ1} atom is also bonded to a C^{δ1} atom, which is part of an isopropyl group (CH(CH₃)₂, labeled H^{δ13}).

Residue probability: 0.669
Residue probability confidence: 1.000

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	173.357	175.926	2.710	0.000	0.000
CA 3.5.1	60.544	61.717	4.152	0.303	1.000
CB 3.5.2	39.532	38.702	3.945	0.750	1.000
CG1 3.5.3	27.650	27.785	2.037	0.714	1.000
CG2 3.5.4	17.116	17.574	1.928	0.376	1.000
CD1 3.5.5	13.410	13.545	3.646	1.000	1.000
N 3.5.6	123.010	121.467	6.098	0.779	1.000
HA 3.5.7	4.833	4.185	1.403	0.750	1.000
HB 3.5.8	1.646	1.776	0.310	0.875	1.000
HG12 3.5.9	1.807	1.271	0.411	0.625	1.000
HG13 3.5.10	0.846	1.186	0.426	0.714	1.000
HG2 3.5.11	0.841	0.762	0.283	0.750	1.000
HD1 3.5.12	0.624	0.668	0.293	0.434	1.000
H 3.5.13	8.765	8.301	0.685	0.623	1.000

Overall probability: 0.303
Overall confidence: 1.000

Residue	Probability	Confidence
LEU4	0.00	1.00
ILE5	0.43	1.00
LEU6	0.00	1.00

Proton	Expected probability
L4HA	1.00
I5HB	1.00
I5HG12	1.00
I5HG13	1.00
I5HG21	1.00
I5HD11	0.97
I5H	1.00
I5HA	1.00
L6H	1.00
L6HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU4	HA	1.00	0.189	0.00	0.00
ILE5	HA	1.00	0.077	0.00	0.00
ILE5	HB	1.00	0.026	1.00	0.59
ILE5	HG12	1.00	0.187	0.00	0.00
ILE5	HG13	1.00	0.005	1.00	0.15
ILE5	HG21	1.00	0.010	1.00	0.15
ILE5	HD11	0.97	0.227	0.03	0.00
ILE5	H	1.00	0.251	0.00	0.00
LEU6	HA	1.00	0.076	0.00	0.00
LEU6	H	1.00	0.100	0.00	0.00

3.5.2 Detailed Probabilities of ILE5CB:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE5	0.86	1.00
LEU6	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I5HA	1.00
I5HG12	1.00
I5HG13	1.00
I5HG21	1.00
I5HD11	1.00
I5H	1.00
I5HB	1.00
L6H	1.00

NOESY contacts detailed probability

3.5 ILE(5)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE5	HA	1.00	0.006	1.00	0.10
ILE5	HB	1.00	0.014	1.00	1.78
ILE5	HG12	1.00	0.005	1.00	0.27
ILE5	HG13	1.00	0.005	1.00	0.78
ILE5	HG21	1.00	0.000	1.00	0.78
ILE5	HD11	1.00	0.217	0.00	0.00
ILE5	H	1.00	0.001	1.00	0.18
LEU6	H	1.00	0.109	0.00	0.00

3.5.3 Detailed Probabilities of ILE5CG1:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE5	0.71	1.00

Expected NOESY Contacts

Proton	Expected probability
I5HA	1.00
I5HB	1.00
I5HG12	1.00
I5HG21	1.00
I5HD11	1.00
I5H	1.00
I5HG13	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE5	HA	1.00	0.075	0.00	0.00
ILE5	HB	1.00	0.014	1.00	0.28
ILE5	HG12	1.00	0.015	1.00	0.89
ILE5	HG13	1.00	0.012	1.00	3.51
ILE5	HG21	1.00	0.017	1.00	3.51
ILE5	HD11	1.00	0.093	0.00	0.00
ILE5	H	1.00	0.028	1.00	0.09

3.5.4 Detailed Probabilities of ILE5CG2:

Overall probability: 0.376

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE5	0.29	1.00
LEU6	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I5HA	1.00
I5HB	1.00
I5HG12	1.00
I5HG13	1.00
I5HG22	1.00
I5HD11	0.99
I5H	1.00
L6H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE5	HA	1.00	0.020	1.00	0.53
ILE5	HB	1.00	0.017	1.00	1.39
ILE5	HG12	1.00	0.110	0.00	0.00
ILE5	HG13	1.00	0.783	0.00	0.00
ILE5	HG21	1.00	0.788	0.00	0.00
ILE5	HD11	0.99	0.574	0.01	0.00
ILE5	H	1.00	0.404	0.00	0.00
LEU6	H	0.98	0.002	1.00	0.51

3.5.5 Detailed Probabilities of ILE5CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE5	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I5HA	0.97
I5HB	1.00
I5HG12	1.00
I5HG13	1.00
I5HG21	0.99
I5HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE5	HA	0.97	0.003	1.00	0.55
ILE5	HB	1.00	0.026	1.00	1.71
ILE5	HG12	1.00	0.007	1.00	2.88
ILE5	HG13	1.00	0.011	1.00	6.14
ILE5	HG21	0.99	0.016	1.00	6.14
ILE5	HD11	1.00	0.001	1.00	90.84
ILE5	H	0.94	0.026	1.00	0.59

3.5.6 Detailed Probabilities of ILE5N:

Overall probability: 0.779

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU4	1.00	1.00
ILE5	0.57	1.00
LEU6	0.90	1.00

Expected NOESY Contacts

Proton	Expected probability
L4HB2	1.00
L4H	1.00
L4HA	1.00
L4HG	0.99
I5HA	1.00
I5HB	1.00
I5HG12	1.00
I5HG13	1.00
I5HG21	1.00
I5H	1.00
L6H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU4	HA	1.00	0.000	1.00	-702003.00
LEU4	HB2	1.00	0.004	1.00	-259686.00
LEU4	HG	0.99	0.010	1.00	-259686.00
LEU4	H	1.00	0.011	1.00	-79576.00
LEU4	HD11	0.53	0.009	1.00	-316736.00
LEU4	HD21	0.63	0.027	1.00	-316736.00
ILE5	HA	1.00	0.009	1.00	-92174.00
ILE5	HB	1.00	0.010	1.00	-253192.00
ILE5	HG12	1.00	0.002	1.00	-110150.00
ILE5	HG13	1.00	0.195	0.00	0.00
ILE5	HG21	1.00	0.190	0.00	0.00
ILE5	H	1.00	0.327	0.00	0.00
ILE5	HD11	0.94	0.027	1.00	-316736.00
LEU6	H	1.00	0.031	0.90	0.00

3.5.7 Detailed Probabilities of ILE5HA:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU4	1.00	1.00
ILE5	0.71	1.00
LEU6	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
L4HA	1.00
I5HB	1.00
I5HG12	1.00
I5HG13	1.00
I5HG21	1.00
I5HD11	0.97
I5H	1.00
I5HA	1.00
L6H	1.00
L6HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU4	HA	1.00	0.007	1.00	0.06
LEU4	HB2	0.60	0.011	1.00	0.12
LEU4	H	0.93	0.002	1.00	-1542108.00
ILE5	HA	1.00	0.077	0.00	0.00
ILE5	HB	1.00	0.006	1.00	0.10
ILE5	HG12	1.00	0.012	1.00	0.14
ILE5	HG13	1.00	0.075	0.00	0.00
ILE5	HG21	1.00	0.020	1.00	0.53
ILE5	HD11	0.97	0.003	1.00	0.55
ILE5	H	1.00	0.009	1.00	-92174.00
LEU6	HA	1.00	0.363	0.00	0.00
LEU6	H	1.00	0.015	1.00	-1116232.00

3.5.8 Detailed Probabilities of ILE5HB:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE5	0.86	1.00
LEU6	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I5HA	1.00
I5HG12	1.00
I5HG13	1.00
I5HG21	1.00
I5HD11	1.00
I5H	1.00
I5HB	1.00
L6H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE5	HA	1.00	0.026	1.00	0.59
ILE5	HB	1.00	0.014	1.00	1.78
ILE5	HG12	1.00	0.419	0.00	0.00
ILE5	HG13	1.00	0.014	1.00	0.28
ILE5	HG21	1.00	0.017	1.00	1.39
ILE5	HD11	1.00	0.026	1.00	1.71
ILE5	H	1.00	0.010	1.00	-253192.00
LEU6	H	1.00	0.004	1.00	-144108.00

3.5.9 Detailed Probabilities of ILE5HG12:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE5	0.57	1.00
LEU6	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I5HA	1.00
I5HB	1.00
I5HG13	1.00
I5HG21	1.00
I5HD11	1.00
I5H	1.00
I5HG12	1.00
L6H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE5	HA	1.00	0.187	0.00	0.00
ILE5	HB	1.00	0.005	1.00	0.27
ILE5	HG12	1.00	0.258	0.00	0.00
ILE5	HG13	1.00	0.015	1.00	0.89
ILE5	HG21	1.00	0.110	0.00	0.00
ILE5	HD11	1.00	0.007	1.00	2.88
ILE5	H	1.00	0.002	1.00	-110150.00
LEU6	H	0.98	0.000	1.00	-76996.00

3.5.10 Detailed Probabilities of ILE5HG13:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE5	0.71	1.00

Expected NOESY Contacts

Proton	Expected probability
I5HA	1.00
I5HB	1.00
I5HG12	1.00
I5HG21	1.00
I5HD11	1.00
I5H	1.00
I5HG13	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE5	HA	1.00	0.005	1.00	0.15
ILE5	HB	1.00	0.005	1.00	0.78
ILE5	HG12	1.00	0.003	1.00	0.92
ILE5	HG13	1.00	0.012	1.00	3.51
ILE5	HG21	1.00	0.783	0.00	0.00
ILE5	HD11	1.00	0.011	1.00	6.14
ILE5	H	1.00	0.195	0.00	0.00

3.5.11 Detailed Probabilities of ILE5HG21:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE5	0.71	1.00
LEU6	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I5HA	1.00
I5HB	1.00
I5HG12	1.00
I5HG13	1.00
I5HG22	1.00
I5HD11	0.99
I5H	1.00
L6H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE5	HA	1.00	0.010	1.00	0.15
ILE5	HB	1.00	0.000	1.00	0.78
ILE5	HG12	1.00	0.008	1.00	0.92
ILE5	HG13	1.00	0.017	1.00	3.51
ILE5	HG21	1.00	0.788	0.00	0.00
ILE5	HD11	0.99	0.016	1.00	6.14
ILE5	H	1.00	0.190	0.00	0.00
LEU6	H	0.98	0.004	1.00	-713415.00

3.5.12 Detailed Probabilities of ILE5HD11:

Overall probability: 0.434

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE5	0.43	1.00

Expected NOESY Contacts

Proton	Expected probability
I5HA	0.97
I5HB	1.00
I5HG12	1.00
I5HG13	1.00
I5HG21	0.99
I5HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE5	HA	0.97	0.227	0.03	0.00
ILE5	HB	1.00	0.217	0.00	0.00
ILE5	HG12	1.00	0.005	1.00	0.55
ILE5	HG13	1.00	0.093	0.00	0.00
ILE5	HG21	0.99	0.574	0.01	0.00
ILE5	HD11	1.00	0.001	1.00	90.84
ILE5	H	0.94	0.027	1.00	-316736.00

3.5.13 Detailed Probabilities of ILE5H:

Overall probability: 0.623

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU4	0.82	1.00
ILE5	0.57	1.00
LEU6	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L4HB2	1.00
L4H	1.00
L4HA	1.00
L4HG	0.99
I5HA	1.00
I5HB	1.00
I5HG12	1.00
I5HG13	1.00
I5HG21	1.00
I5H	1.00
L6H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU4	HA	1.00	0.005	1.00	0.61
LEU4	HB2	1.00	0.014	1.00	0.11
LEU4	HG	0.99	0.039	0.10	0.00
LEU4	H	1.00	0.019	1.00	-121633.00
LEU4	HD11	0.53	0.009	1.00	0.28
ILE5	HA	1.00	0.251	0.00	0.00
ILE5	HB	1.00	0.001	1.00	0.18
ILE5	HG12	1.00	0.002	1.00	0.08
ILE5	HG13	1.00	0.028	1.00	0.09
ILE5	HG21	1.00	0.404	0.00	0.00
ILE5	H	1.00	0.327	0.00	0.00
ILE5	HD11	0.94	0.026	1.00	0.59
LEU6	H	1.00	0.169	0.00	0.00

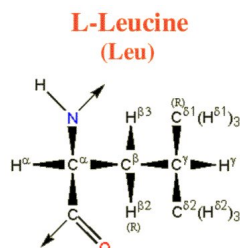


Figure 6: Image from the BMRB

Residue probability: 0.823
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.795	177.056	1.929	0.000	0.000
CA 3.6.1	53.000	55.735	3.802	0.760	1.000
CB 3.6.2	44.528	42.389	3.750	0.956	1.000
CG 3.6.3	27.906	26.892	3.086	0.875	1.000
CD1 3.6.4	25.511	24.837	3.657	1.000	1.000
CD2 3.6.5	25.367	24.201	3.117	1.000	1.000
N 3.6.6	129.320	121.785	4.943	0.873	1.000
HA 3.6.7	5.346	4.315	0.840	0.818	1.000
HB2 3.6.8	1.508	1.601	0.373	0.750	1.000
HB3 3.6.9	1.458	1.508	0.398	0.678	1.000
HG 3.6.10	1.520	1.510	0.340	0.577	1.000
HD1 3.6.11	0.715	0.739	0.294	0.857	1.000
HD2 3.6.12	0.735	0.727	0.421	0.857	1.000
H 3.6.13	9.235	8.237	0.647	0.701	1.000

3.6.1 Detailed Probabilities of LEU6CA:

Overall probability: 0.760
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE5	0.00	1.00
LEU6	0.80	1.00
ILE7	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I5HA	1.00
L6HB2	1.00
L6HB3	1.00
L6HG	1.00
L6HD11	0.99
L6HD21	0.99
L6H	1.00
L6HA	1.00
I7H	1.00
I7HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE5	HA	1.00	0.363	0.00	0.00
LEU6	HA	1.00	0.001	1.00	1.99
LEU6	HB2	1.00	0.029	1.00	0.47
LEU6	HB3	1.00	0.021	1.00	0.47
LEU6	HG	1.00	0.041	0.00	0.00
LEU6	HD11	0.99	0.011	1.00	0.77
LEU6	HD21	0.99	0.009	1.00	0.77
LEU6	H	1.00	0.034	0.60	0.00
ILE7	HA	1.00	0.015	1.00	0.06
ILE7	H	1.00	0.005	1.00	0.95

3.6.2 Detailed Probabilities of LEU6CB:

Overall probability: 0.956

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU6	0.94	1.00
ILE7	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L6HA	1.00
L6HB3	1.00
L6HG	1.00
L6HD11	1.00
L6HD21	1.00
L6H	1.00
L6HB2	1.00
I7H	1.00

NOESY contacts detailed probability

3.6 LEU(6)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU6	HA	1.00	0.003	1.00	0.16
LEU6	HB2	1.00	0.022	1.00	1.87
LEU6	HB3	1.00	0.028	1.00	1.87
LEU6	HG	1.00	0.034	0.60	0.00
LEU6	HD11	1.00	0.029	1.00	0.83
LEU6	HD21	1.00	0.009	1.00	0.83
LEU6	H	1.00	0.001	1.00	0.18
ILE7	H	1.00	0.008	1.00	0.07
ILE7	HA	0.60	0.019	1.00	0.05

3.6.3 Detailed Probabilities of LEU6CG:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU6	0.86	1.00
ILE7	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L6HA	1.00
L6HB2	1.00
L6HB3	1.00
L6HD11	1.00
L6HD21	1.00
L6H	1.00
L6HG	1.00
I7H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU6	HA	1.00	0.007	1.00	0.21
LEU6	HB2	1.00	0.018	1.00	8.86
LEU6	HB3	1.00	0.068	0.00	0.00
LEU6	HG	1.00	0.006	1.00	8.86
LEU6	HD11	1.00	0.011	1.00	1.98
LEU6	HD21	1.00	0.009	1.00	1.98
LEU6	H	1.00	0.007	1.00	0.22
ILE7	H	0.99	0.001	1.00	0.07

3.6.4 Detailed Probabilities of LEU6CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU6	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L6HA	0.99
L6HB2	1.00
L6HB3	1.00
L6HG	1.00
L6HD12	1.00
L6HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU6	HA	0.99	0.004	1.00	0.92
LEU6	HB2	1.00	0.004	1.00	3.61
LEU6	HB3	1.00	0.017	1.00	3.93
LEU6	HG	1.00	0.008	1.00	3.61
LEU6	HD11	1.00	0.012	1.00	164.25
LEU6	HD21	1.00	0.008	1.00	164.25
LEU6	H	0.86	0.014	1.00	0.42

3.6.5 Detailed Probabilities of LEU6CD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU6	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L6HA	0.99
L6HB2	1.00
L6HB3	1.00
L6HG	1.00
L6HD11	1.00
L6HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU6	HA	0.99	0.004	1.00	0.92
LEU6	HB2	1.00	0.004	1.00	3.61
LEU6	HB3	1.00	0.017	1.00	3.93
LEU6	HG	1.00	0.008	1.00	3.61
LEU6	HD11	1.00	0.012	1.00	164.25
LEU6	HD21	1.00	0.008	1.00	164.25
LEU6	H	0.85	0.014	1.00	0.42

3.6.6 Detailed Probabilities of LEU6N:

Overall probability: 0.873

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE5	0.83	1.00
LEU6	0.87	1.00
ILE7	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I5HG21	0.98
I5HG12	0.98
I5HA	1.00
I5HB	1.00
I5H	1.00
L6HA	1.00
L6HB2	1.00
L6HB3	1.00
L6HG	1.00
L6H	1.00
I7H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE5	HA	1.00	0.015	1.00	-1116232.00
ILE5	HB	1.00	0.004	1.00	-144108.00
ILE5	HG12	0.98	0.000	1.00	-76996.00
ILE5	HG21	0.98	0.004	1.00	-713415.00
ILE5	H	1.00	0.169	0.00	0.00
ILE5	HG13	0.93	0.009	1.00	-713415.00
LEU6	HA	1.00	0.005	1.00	-250400.00
LEU6	HB2	1.00	0.011	1.00	-701933.00
LEU6	HB3	1.00	0.039	0.10	0.00
LEU6	HG	1.00	0.023	1.00	-701933.00
LEU6	H	1.00	0.001	1.00	-3628454.00
LEU6	HD11	0.88	0.018	1.00	-563924.00
LEU6	HD21	0.87	0.002	1.00	-563924.00
ILE7	H	1.00	0.003	1.00	-98177.00
ILE7	HA	0.93	0.011	1.00	-90837.00

3.6.7 Detailed Probabilities of LEU6HA:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE5	0.00	1.00
LEU6	1.00	1.00
ILE7	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
I5HA	1.00
L6HB2	1.00
L6HB3	1.00
L6HG	1.00
L6HD11	0.99
L6HD21	0.99
L6H	1.00
L6HA	1.00
I7H	1.00
I7HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE5	HA	1.00	0.076	0.00	0.00
LEU6	HA	1.00	0.001	1.00	1.99
LEU6	HB2	1.00	0.003	1.00	0.16
LEU6	HB3	1.00	0.001	1.00	0.21
LEU6	HG	1.00	0.007	1.00	0.21
LEU6	HD11	0.99	0.004	1.00	0.92
LEU6	HD21	0.99	0.004	1.00	0.92
LEU6	H	1.00	0.005	1.00	-250400.00
ILE7	HA	1.00	0.162	0.00	0.00
ILE7	H	1.00	0.000	1.00	-1300162.00
ILE7	HG13	0.63	0.009	1.00	0.06

3.6.8 Detailed Probabilities of LEU6HB2:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU6	0.86	1.00
ILE7	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L6HA	1.00
L6HB3	1.00
L6HG	1.00
L6HD11	1.00
L6HD21	1.00
L6H	1.00
L6HB2	1.00
I7H	1.00

NOESY contacts detailed probability

3.6 LEU(6)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU6	HA	1.00	0.029	1.00	0.47
LEU6	HB2	1.00	0.022	1.00	1.87
LEU6	HB3	1.00	2.455	0.00	0.00
LEU6	HG	1.00	0.018	1.00	8.86
LEU6	HD11	1.00	0.004	1.00	3.61
LEU6	HD21	1.00	0.004	1.00	3.61
LEU6	H	1.00	0.011	1.00	-701933.00
ILE7	H	1.00	0.042	0.00	0.00

3.6.9 Detailed Probabilities of LEU6HB3:

Overall probability: 0.678

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU6	0.59	1.00
ILE7	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L6HA	1.00
L6HB2	1.00
L6HG	1.00
L6HD11	1.00
L6HD21	1.00
L6H	1.00
L6HB3	1.00
I7H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU6	HA	1.00	0.021	1.00	0.47
LEU6	HB2	1.00	0.028	1.00	1.87
LEU6	HB3	1.00	2.405	0.00	0.00
LEU6	HG	1.00	0.068	0.00	0.00
LEU6	HD11	1.00	0.017	1.00	3.93
LEU6	HD21	1.00	0.017	1.00	3.93
LEU6	H	1.00	0.039	0.10	0.00
ILE7	H	1.00	0.008	1.00	-503766.00
ILE7	HA	0.92	0.010	1.00	0.21

3.6.10 Detailed Probabilities of LEU6HG:

Overall probability: 0.577

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU6	0.66	1.00
ILE7	0.01	1.00

Expected NOESY Contacts

Proton	Expected probability
L6HA	1.00
L6HB2	1.00
L6HB3	1.00
L6HD11	1.00
L6HD21	1.00
L6H	1.00
L6HG	1.00
I7H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU6	HA	1.00	0.041	0.00	0.00
LEU6	HB2	1.00	0.034	0.60	0.00
LEU6	HB3	1.00	2.467	0.00	0.00
LEU6	HG	1.00	0.006	1.00	8.86
LEU6	HD11	1.00	0.008	1.00	3.61
LEU6	HD21	1.00	0.008	1.00	3.61
LEU6	H	1.00	0.023	1.00	-701933.00
ILE7	H	0.99	0.054	0.01	0.00

3.6.11 Detailed Probabilities of LEU6HD11:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU6	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
L6HA	0.99
L6HB2	1.00
L6HB3	1.00
L6HG	1.00
L6HD12	1.00
L6HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU6	HA	0.99	0.011	1.00	0.77
LEU6	HB2	1.00	0.029	1.00	0.83
LEU6	HB3	1.00	1.662	0.00	0.00
LEU6	HG	1.00	0.011	1.00	1.98
LEU6	HD11	1.00	0.012	1.00	164.25
LEU6	HD21	1.00	0.012	1.00	164.25
LEU6	H	0.86	0.018	1.00	-563924.00

3.6.12 Detailed Probabilities of LEU6HD21:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU6	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
L6HA	0.99
L6HB2	1.00
L6HB3	1.00
L6HG	1.00
L6HD11	1.00
L6HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU6	HA	0.99	0.009	1.00	0.77
LEU6	HB2	1.00	0.009	1.00	0.83
LEU6	HB3	1.00	1.682	0.00	0.00
LEU6	HG	1.00	0.009	1.00	1.98
LEU6	HD11	1.00	0.008	1.00	164.25
LEU6	HD21	1.00	0.008	1.00	164.25
LEU6	H	0.85	0.002	1.00	-563924.00

3.6.13 Detailed Probabilities of LEU6H:

Overall probability: 0.701

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE5	0.49	1.00
LEU6	0.94	1.00
ILE7	0.30	1.00

Expected NOESY Contacts

Proton	Expected probability
I5HG21	0.98
I5HG12	0.98
I5HA	1.00
I5HB	1.00
I5H	1.00
L6HA	1.00
L6HB2	1.00
L6HB3	1.00
L6HG	1.00
L6H	1.00
I7H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE5	HA	1.00	0.100	0.00	0.00
ILE5	HB	1.00	0.109	0.00	0.00
ILE5	HG12	0.98	0.472	0.02	0.00
ILE5	HG21	0.98	0.002	1.00	0.51
ILE5	H	1.00	0.031	0.90	0.00
ILE5	HG13	0.93	0.028	1.00	0.05
LEU6	HA	1.00	0.034	0.60	0.00
LEU6	HB2	1.00	0.001	1.00	0.18
LEU6	HB3	1.00	0.003	1.00	0.23
LEU6	HG	1.00	0.007	1.00	0.22
LEU6	H	1.00	0.001	1.00	-3628454.00
LEU6	HD11	0.88	0.014	1.00	0.42
LEU6	HD21	0.87	0.014	1.00	0.42
ILE7	H	1.00	0.037	0.30	0.00

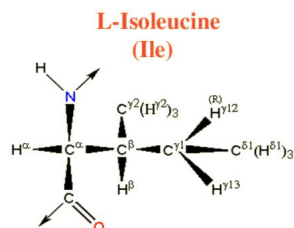


Figure 7: Image from the BMRB

Residue probability: 0.891
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	173.819	175.926	2.710	0.000	0.000
CA 3.7.1	58.215	61.717	4.152	0.909	1.000
CB 3.7.2	40.154	38.702	3.945	0.875	1.000
CG1 3.7.3	27.098	27.785	2.037	0.880	1.000
CG2 3.7.4	16.613	17.574	1.928	1.000	1.000
CD1 3.7.5	14.164	13.545	3.646	1.000	1.000
N 3.7.6	120.746	121.467	6.098	0.737	1.000
HA 3.7.7	5.181	4.185	1.403	0.833	1.000
HB 3.7.8	1.892	1.776	0.310	1.000	1.000
HG12 3.7.9	1.459	1.271	0.411	0.750	1.000
HG13 3.7.10	1.253	1.186	0.426	0.880	1.000
HG2 3.7.11	0.744	0.762	0.283	0.875	1.000
HD1 3.7.12	0.767	0.668	0.293	0.849	1.000
H 3.7.13	8.931	8.301	0.685	1.000	1.000

3.7.1 Detailed Probabilities of ILE7CA:

Overall probability: 0.909
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU6	0.50	1.00
ILE7	1.00	1.00
ASN8	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L6HA	1.00
I7HB	1.00
I7HG12	1.00
I7HG13	1.00
I7HG21	1.00
I7HD11	0.97
I7H	1.00
I7HA	1.00
N8H	1.00
N8HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU6	HA	1.00	0.162	0.00	0.00
LEU6	HB3	0.92	0.010	1.00	0.21
ILE7	HA	1.00	0.003	1.00	2.09
ILE7	HB	1.00	0.014	1.00	0.31
ILE7	HG12	1.00	0.009	1.00	0.21
ILE7	HG13	1.00	0.001	1.00	0.20
ILE7	HG21	1.00	0.008	1.00	0.96
ILE7	HD11	0.97	0.015	1.00	0.96
ILE7	H	1.00	0.003	1.00	0.21
ASN8	HA	1.00	0.017	1.00	0.09
ASN8	H	1.00	0.007	1.00	0.72

3.7.2 Detailed Probabilities of ILE7CB:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE7	0.86	1.00
ASN8	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I7HA	1.00
I7HG12	1.00
I7HG13	1.00
I7HG21	1.00
I7HD11	1.00
I7H	1.00
I7HB	1.00
N8H	1.00

NOESY contacts detailed probability

3.7 ILE(7)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE7	HA	1.00	0.003	1.00	0.18
ILE7	HB	1.00	0.006	1.00	2.28
ILE7	HG12	1.00	0.198	0.00	0.00
ILE7	HG13	1.00	0.008	1.00	0.27
ILE7	HG21	1.00	0.001	1.00	1.28
ILE7	HD11	1.00	0.024	1.00	1.28
ILE7	H	1.00	0.004	1.00	0.36
ASN8	H	1.00	0.004	1.00	0.08

3.7.3 Detailed Probabilities of ILE7CG1:

Overall probability: 0.880

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE7	1.00	1.00
ASN8	0.04	1.00

Expected NOESY Contacts

Proton	Expected probability
I7HA	1.00
I7HB	1.00
I7HG12	1.00
I7HG21	1.00
I7HD11	1.00
I7H	1.00
I7HG13	1.00
N8H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE7	HA	1.00	0.006	1.00	0.21
ILE7	HB	1.00	0.010	1.00	0.60
ILE7	HG12	1.00	0.003	1.00	2.13
ILE7	HG13	1.00	0.003	1.00	5.04
ILE7	HG21	1.00	0.005	1.00	2.11
ILE7	HD11	1.00	0.018	1.00	2.11
ILE7	H	1.00	0.003	1.00	0.20
ASN8	H	0.96	0.175	0.04	0.00

3.7.4 Detailed Probabilities of ILE7CG2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE7	1.00	1.00
ASN8	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I7HA	1.00
I7HB	1.00
I7HG12	1.00
I7HG13	1.00
I7HG22	1.00
I7HD11	0.99
I7H	1.00
N8H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE7	HA	1.00	0.000	1.00	0.71
ILE7	HB	1.00	0.009	1.00	1.38
ILE7	HG12	1.00	0.002	1.00	0.72
ILE7	HG13	1.00	0.001	1.00	0.53
ILE7	HG21	1.00	0.000	1.00	28.78
ILE7	HD11	0.99	0.023	1.00	28.78
ILE7	H	1.00	0.001	1.00	0.27
ASN8	H	0.98	0.005	1.00	0.41
ASN8	HA	0.62	0.003	1.00	0.09

3.7.5 Detailed Probabilities of ILE7CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE7	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I7HA	0.97
I7HB	1.00
I7HG12	1.00
I7HG13	1.00
I7HG21	0.99
I7HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE7	HA	0.97	0.004	1.00	0.43
ILE7	HB	1.00	0.010	1.00	0.98
ILE7	HG12	1.00	0.000	1.00	1.43
ILE7	HG13	1.00	0.000	1.00	1.15
ILE7	HG21	0.99	0.020	1.00	50.00
ILE7	HD11	1.00	0.003	1.00	50.00
ILE7	H	0.94	0.004	1.00	0.20

3.7.6 Detailed Probabilities of ILE7N:

Overall probability: 0.737

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU6	0.62	1.00
ILE7	1.00	1.00
ASN8	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L6HB2	1.00
L6H	1.00
L6HB3	1.00
L6HA	1.00
L6HG	0.99
I7HA	1.00
I7HB	1.00
I7HG12	1.00
I7HG13	1.00
I7HG21	1.00
I7H	1.00
N8H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU6	HA	1.00	0.000	1.00	-1300162.00
LEU6	HB2	1.00	0.042	0.00	0.00
LEU6	HB3	1.00	0.008	1.00	-503766.00
LEU6	HG	0.99	0.054	0.01	0.00
LEU6	H	1.00	0.037	0.30	0.00
LEU6	HD11	0.53	0.018	1.00	-930878.00
LEU6	HD21	0.63	0.002	1.00	-930878.00
ILE7	HA	1.00	0.006	1.00	-166467.00
ILE7	HB	1.00	0.004	1.00	-466593.00
ILE7	HG12	1.00	0.007	1.00	-503766.00
ILE7	HG13	1.00	0.001	1.00	-235037.00
ILE7	HG21	1.00	0.011	1.00	-930878.00
ILE7	H	1.00	0.004	1.00	-3583773.00
ASN8	H	1.00	0.157	0.00	0.00

3.7.7 Detailed Probabilities of ILE7HA:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU6	1.00	1.00
ILE7	0.86	1.00
ASN8	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
L6HA	1.00
I7HB	1.00
I7HG12	1.00
I7HG13	1.00
I7HG21	1.00
I7HD11	0.97
I7H	1.00
I7HA	1.00
N8H	1.00
N8HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU6	HA	1.00	0.015	1.00	0.06
LEU6	HB2	0.60	0.019	1.00	0.05
LEU6	H	0.93	0.011	1.00	-90837.00
ILE7	HA	1.00	0.003	1.00	2.09
ILE7	HB	1.00	0.003	1.00	0.18
ILE7	HG12	1.00	0.434	0.00	0.00
ILE7	HG13	1.00	0.006	1.00	0.21
ILE7	HG21	1.00	0.000	1.00	0.71
ILE7	HD11	0.97	0.004	1.00	0.43
ILE7	H	1.00	0.006	1.00	-166467.00
ASN8	HA	1.00	0.061	0.00	0.00
ASN8	H	1.00	0.003	1.00	-1319913.00

3.7.8 Detailed Probabilities of ILE7HB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE7	1.00	1.00
ASN8	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I7HA	1.00
I7HG12	1.00
I7HG13	1.00
I7HG21	1.00
I7HD11	1.00
I7H	1.00
I7HB	1.00
N8H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE7	HA	1.00	0.014	1.00	0.31
ILE7	HB	1.00	0.006	1.00	2.28
ILE7	HG12	1.00	0.004	1.00	0.65
ILE7	HG13	1.00	0.010	1.00	0.60
ILE7	HG21	1.00	0.009	1.00	1.38
ILE7	HD11	1.00	0.010	1.00	0.98
ILE7	H	1.00	0.004	1.00	-466593.00
ASN8	H	1.00	0.016	1.00	-157710.00

3.7.9 Detailed Probabilities of ILE7HG12:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE7	0.71	1.00
ASN8	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I7HA	1.00
I7HB	1.00
I7HG13	1.00
I7HG21	1.00
I7HD11	1.00
I7H	1.00
I7HG12	1.00
N8H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE7	HA	1.00	0.009	1.00	0.21
ILE7	HB	1.00	0.198	0.00	0.00
ILE7	HG12	1.00	0.201	0.00	0.00
ILE7	HG13	1.00	0.003	1.00	2.13
ILE7	HG21	1.00	0.002	1.00	0.72
ILE7	HD11	1.00	0.000	1.00	1.43
ILE7	H	1.00	0.007	1.00	-503766.00
ASN8	H	0.98	0.003	1.00	-180812.00

3.7.10 Detailed Probabilities of ILE7HG13:

Overall probability: 0.880

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE7	1.00	1.00
ASN8	0.04	1.00

Expected NOESY Contacts

Proton	Expected probability
I7HA	1.00
I7HB	1.00
I7HG12	1.00
I7HG21	1.00
I7HD11	1.00
I7H	1.00
I7HG13	1.00
N8H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE7	HA	1.00	0.001	1.00	0.20
ILE7	HB	1.00	0.008	1.00	0.27
ILE7	HG12	1.00	0.005	1.00	2.06
ILE7	HG13	1.00	0.003	1.00	5.04
ILE7	HG21	1.00	0.001	1.00	0.53
ILE7	HD11	1.00	0.000	1.00	1.15
ILE7	H	1.00	0.001	1.00	-235037.00
ASN8	H	0.96	0.104	0.04	0.00

3.7.11 Detailed Probabilities of ILE7HG21:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE7	0.86	1.00
ASN8	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I7HA	1.00
I7HB	1.00
I7HG12	1.00
I7HG13	1.00
I7HG22	1.00
I7HD11	0.99
I7H	1.00
N8H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE7	HA	1.00	0.008	1.00	0.96
ILE7	HB	1.00	0.001	1.00	1.28
ILE7	HG12	1.00	0.514	0.00	0.00
ILE7	HG13	1.00	0.005	1.00	2.11
ILE7	HG21	1.00	0.000	1.00	28.78
ILE7	HD11	0.99	0.020	1.00	50.00
ILE7	H	1.00	0.011	1.00	-930878.00
ASN8	H	0.98	0.009	1.00	-876972.00

3.7.12 Detailed Probabilities of ILE7HD11:

Overall probability: 0.849

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE7	0.85	1.00

Expected NOESY Contacts

Proton	Expected probability
I7HA	0.97
I7HB	1.00
I7HG12	1.00
I7HG13	1.00
I7HG21	0.99
I7HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE7	HA	0.97	0.015	1.00	0.96
ILE7	HB	1.00	0.024	1.00	1.28
ILE7	HG12	1.00	0.491	0.00	0.00
ILE7	HG13	1.00	0.018	1.00	2.11
ILE7	HG21	0.99	0.023	1.00	28.78
ILE7	HD11	1.00	0.003	1.00	50.00
ILE7	H	0.94	0.034	0.94	0.00

3.7.13 Detailed Probabilities of ILE7H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU6	1.00	1.00
ILE7	1.00	1.00
ASN8	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L6HB2	1.00
L6H	1.00
L6HB3	1.00
L6HA	1.00
L6HG	0.99
I7HA	1.00
I7HB	1.00
I7HG12	1.00
I7HG13	1.00
I7HG21	1.00
I7H	1.00
N8H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU6	HA	1.00	0.005	1.00	0.95
LEU6	HB2	1.00	0.008	1.00	0.07
LEU6	HB3	1.00	0.009	1.00	0.06
LEU6	HG	0.99	0.001	1.00	0.07
LEU6	H	1.00	0.003	1.00	-98177.00
LEU6	HD11	0.53	0.003	1.00	0.32
LEU6	HD21	0.63	0.003	1.00	0.32
ILE7	HA	1.00	0.003	1.00	0.21
ILE7	HB	1.00	0.004	1.00	0.36
ILE7	HG12	1.00	0.002	1.00	0.18
ILE7	HG13	1.00	0.003	1.00	0.20
ILE7	HG21	1.00	0.001	1.00	0.27
ILE7	H	1.00	0.004	1.00	-3583773.00
ILE7	HD11	0.94	0.004	1.00	0.20
ASN8	H	1.00	0.011	1.00	-84367.00

3.8 ASN(8)

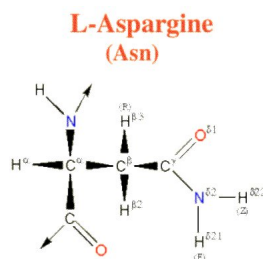


Figure 8: Image from the BMRB

Residue probability: 0.894
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	176.478	175.315	1.862	0.000	0.000
CA 3.8.1	51.104	53.674	5.429	0.889	1.000
CB 3.8.2	42.582	38.785	5.449	1.000	1.000
N 3.8.3	125.539	118.907	6.480	0.839	1.000
ND2 3.8.4	107.513	112.932	14.355	1.000	1.000
HA 3.8.5	5.902	4.658	0.371	0.900	1.000
HB2 3.8.6	2.891	2.800	0.341	1.000	1.000
HB3 3.8.7	2.273	2.739	0.364	1.000	1.000
H 3.8.8	8.634	8.328	0.633	0.674	1.000
HD21 3.8.9	7.368	7.343	1.188	0.837	1.000
HD22 3.8.10	6.251	7.145	1.184	0.800	1.000

3.8.1 Detailed Probabilities of ASN8CA:

Overall probability: 0.889
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE7	0.00	1.00
ASN8	1.00	1.00
THR9	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I7HA	1.00
N8HB2	1.00
N8HB3	1.00
N8H	1.00
N8HD21	1.00
N8HD22	1.00
N8HA	1.00
T9HA	1.00
T9H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE7	HA	1.00	0.061	0.00	0.00
ASN8	HA	1.00	0.000	1.00	2.06
ASN8	HB2	1.00	0.006	1.00	0.26
ASN8	HB3	1.00	0.000	1.00	0.31
ASN8	H	1.00	0.009	1.00	0.17
ASN8	HD21	1.00	0.003	1.00	0.36
ASN8	HD22	1.00	0.001	1.00	0.18
THR9	HA	1.00	0.005	1.00	0.11
THR9	H	1.00	0.008	1.00	1.01

3.8.2 Detailed Probabilities of ASN8CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN8	1.00	1.00
THR9	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N8HA	1.00
N8HB2	1.00
N8H	1.00
N8HD21	1.00
N8HD22	1.00
N8HB3	1.00
T9H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN8	HA	1.00	0.002	1.00	0.30
ASN8	HB2	1.00	0.000	1.00	1.24
ASN8	HB3	1.00	0.003	1.00	1.41
ASN8	H	1.00	0.003	1.00	0.24
ASN8	HD21	1.00	0.007	1.00	0.15
ASN8	HD22	1.00	0.007	1.00	0.08
THR9	H	1.00	0.010	1.00	0.10

3.8.3 Detailed Probabilities of ASN8N:

Overall probability: 0.839

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE7	0.84	1.00
ASN8	0.80	1.00
THR9	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I7H	1.00
I7HG23	0.98
I7HB	1.00
I7HG13	0.96
I7HA	1.00
I7HG12	0.98
N8HA	1.00
N8HB2	1.00
N8HB3	1.00
N8HD21	0.98
N8H	1.00
T9H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE7	HA	1.00	0.003	1.00	-1319913.00
ILE7	HB	1.00	0.016	1.00	-157710.00
ILE7	HG12	0.98	0.003	1.00	-180812.00
ILE7	HG13	0.96	0.104	0.04	0.00
ILE7	HG21	0.99	0.009	1.00	-876972.00
ILE7	H	1.00	0.011	1.00	-84367.00
ASN8	HA	1.00	0.000	1.00	-236349.00
ASN8	HB2	1.00	0.001	1.00	-413898.00
ASN8	HB3	1.00	0.006	1.00	-285758.00
ASN8	H	1.00	0.004	1.00	-3466320.00
ASN8	HD21	0.98	0.684	0.02	0.00
THR9	H	1.00	0.008	1.00	-80144.00

3.8.4 Detailed Probabilities of ASN8ND2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN8	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N8HA	1.00
N8HB2	1.00
N8HB3	1.00
N8HD21	1.00
N8HD22	1.00

NOESY contacts detailed probability

3.8 ASN(8)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN8	HA	1.00	0.003	1.00	-253123.00
ASN8	HB2	1.00	0.001	1.00	-162177.00
ASN8	HB3	1.00	0.008	1.00	-139723.00
ASN8	HD21	1.00	0.002	1.00	-2307874.00
ASN8	HD22	1.00	0.001	1.00	-2806614.00

3.8.5 Detailed Probabilities of ASN8HA:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE7	1.00	1.00
ASN8	1.00	1.00
THR9	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
I7HA	1.00
N8HB2	1.00
N8HB3	1.00
N8H	1.00
N8HD21	1.00
N8HD22	1.00
N8HA	1.00
T9HA	1.00
T9H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE7	HA	1.00	0.017	1.00	0.09
ILE7	HG21	0.63	0.003	1.00	0.09
ASN8	HA	1.00	0.000	1.00	2.06
ASN8	HB2	1.00	0.006	1.00	0.21
ASN8	HB3	1.00	0.002	1.00	0.30
ASN8	H	1.00	0.000	1.00	-236349.00
ASN8	HD21	1.00	0.002	1.00	-366931.00
ASN8	HD22	1.00	0.003	1.00	-253123.00
THR9	HA	1.00	0.098	0.00	0.00
THR9	H	1.00	0.001	1.00	-1924204.00

3.8.6 Detailed Probabilities of ASN8HB2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN8	1.00	1.00
THR9	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N8HA	1.00
N8HB3	1.00
N8H	1.00
N8HD21	1.00
N8HD22	1.00
N8HB2	1.00
T9H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN8	HA	1.00	0.006	1.00	0.26
ASN8	HB2	1.00	0.026	1.00	220.78
ASN8	HB3	1.00	0.000	1.00	1.24
ASN8	H	1.00	0.001	1.00	-413898.00
ASN8	HD21	1.00	0.001	1.00	-201164.00
ASN8	HD22	1.00	0.001	1.00	-162177.00
THR9	H	1.00	0.010	1.00	-238083.00

3.8.7 Detailed Probabilities of ASN8HB3:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN8	1.00	1.00
THR9	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N8HA	1.00
N8HB2	1.00
N8H	1.00
N8HD21	1.00
N8HD22	1.00
N8HB3	1.00
T9H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN8	HA	1.00	0.000	1.00	0.31
ASN8	HB2	1.00	0.000	1.00	0.99
ASN8	HB3	1.00	0.003	1.00	1.41
ASN8	H	1.00	0.006	1.00	-285758.00
ASN8	HD21	1.00	0.003	1.00	-174920.00
ASN8	HD22	1.00	0.008	1.00	-139723.00
THR9	H	1.00	0.004	1.00	-278457.00

3.8.8 Detailed Probabilities of ASN8H:

Overall probability: 0.674

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE7	0.51	1.00
ASN8	0.80	1.00
THR9	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I7H	1.00
I7HG23	0.98
I7HB	1.00
I7HG13	0.96
I7HA	1.00
I7HG12	0.98
N8HA	1.00
N8HB2	1.00
N8HB3	1.00
N8HD21	0.98
N8H	1.00
T9H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE7	HA	1.00	0.007	1.00	0.72
ILE7	HB	1.00	0.004	1.00	0.08
ILE7	HG12	0.98	0.299	0.02	0.00
ILE7	HG13	0.96	0.175	0.04	0.00
ILE7	HG21	0.99	0.005	1.00	0.41
ILE7	H	1.00	0.157	0.00	0.00
ASN8	HA	1.00	0.009	1.00	0.17
ASN8	HB2	1.00	0.004	1.00	0.20
ASN8	HB3	1.00	0.003	1.00	0.24
ASN8	H	1.00	0.004	1.00	-3466320.00
ASN8	HD21	0.98	0.181	0.02	0.00
THR9	H	1.00	0.000	1.00	-141703.00

3.8.9 Detailed Probabilities of ASN8HD21:

Overall probability: 0.837

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN8	0.84	1.00

Expected NOESY Contacts

Proton	Expected probability
N8HA	1.00
N8HB2	1.00
N8HB3	1.00
N8H	0.98
N8HD22	1.00
N8HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN8	HA	1.00	0.003	1.00	0.36
ASN8	HB2	1.00	0.002	1.00	0.14
ASN8	HB3	1.00	0.007	1.00	0.15
ASN8	H	0.98	0.684	0.02	0.00
ASN8	HD21	1.00	0.003	1.00	-2375694.00
ASN8	HD22	1.00	0.002	1.00	-2307874.00

3.8.10 Detailed Probabilities of ASN8HD22:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN8	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
N8HA	1.00
N8HB2	1.00
N8HB3	1.00
N8HD21	1.00
N8HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN8	HA	1.00	0.001	1.00	0.18
ASN8	HB2	1.00	0.355	0.00	0.00
ASN8	HB3	1.00	0.007	1.00	0.08
ASN8	HD21	1.00	0.000	1.00	-2232060.00
ASN8	HD22	1.00	0.001	1.00	-2806614.00

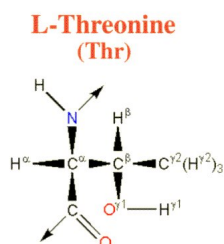


Figure 9: Image from the BMRB

Residue probability: 0.849
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	170.114	174.627	1.788	0.000	0.000
CA 3.9.1	60.689	62.330	4.136	0.575	1.000
CB 3.9.2	67.766	69.395	4.500	1.000	1.000
CG2 3.9.3	19.209	21.588	1.595	0.600	1.000
N 3.9.4	118.493	115.370	5.913	1.000	1.000
HA 3.9.5	4.739	4.461	0.626	1.000	1.000
HB 3.9.6	4.321	4.172	0.855	1.000	1.000
HG2 3.9.7	0.863	1.134	0.349	0.650	1.000
H 3.9.8	8.044	8.272	1.597	0.818	1.000
HG1 3.9.9	6.178	5.002	1.472	1.000	1.000

3.9.1 Detailed Probabilities of THR9CA:

Overall probability: 0.575
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN8	0.00	1.00
THR9	0.72	1.00
ASN10	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
N8HA	1.00
T9HB	1.00
T9HG21	1.00
T9H	1.00
T9HG1	1.00
T9HA	1.00
N10H	1.00
N10HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN8	HA	1.00	0.098	0.00	0.00
THR9	HA	1.00	0.008	1.00	1.28
THR9	HB	1.00	0.024	1.00	0.28
THR9	HG21	1.00	0.034	0.60	0.00
THR9	H	1.00	0.046	0.00	0.00
THR9	HG1	1.00	0.008	1.00	0.59
ASN10	HA	1.00	0.002	1.00	0.49
ASN10	H	1.00	0.124	0.00	0.00

3.9.2 Detailed Probabilities of THR9CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
THR9	1.00	1.00
ASN10	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
T9HA	1.00
T9HG21	1.00
T9H	1.00
T9HG1	1.00
T9HB	1.00
N10H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR9	HA	1.00	0.018	1.00	0.56
THR9	HB	1.00	0.001	1.00	2.03
THR9	HG21	1.00	0.004	1.00	1.06
THR9	H	1.00	0.005	1.00	0.10
THR9	HG1	1.00	0.013	1.00	0.87
ASN10	H	1.00	0.001	1.00	0.26

3.9.3 Detailed Probabilities of THR9CG2:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
THR9	0.60	1.00

Expected NOESY Contacts

Proton	Expected probability
T9HA	1.00
T9HB	1.00
T9HG22	1.00
T9H	1.00
T9HG1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR9	HA	1.00	0.007	1.00	0.34
THR9	HB	1.00	0.003	1.00	1.04
THR9	HG21	1.00	0.103	0.00	0.00
THR9	H	1.00	0.200	0.00	0.00
THR9	HG1	1.00	0.013	1.00	0.48

3.9.4 Detailed Probabilities of THR9N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN8	1.00	1.00
THR9	1.00	1.00
ASN10	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N8H	1.00
N8HA	1.00
N8HB3	1.00
N8HB2	1.00
T9HA	1.00
T9HB	1.00
T9HG21	1.00
T9HG1	1.00
T9H	1.00
N10H	1.00

NOESY contacts detailed probability

3.9 THR(9)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN8	HA	1.00	0.001	1.00	-1924204.00
ASN8	HB2	1.00	0.010	1.00	-238083.00
ASN8	HB3	1.00	0.004	1.00	-278457.00
ASN8	H	1.00	0.000	1.00	-141703.00
ASN8	HD21	0.70	0.002	1.00	-303238.00
THR9	HA	1.00	0.011	1.00	-578376.00
THR9	HB	1.00	0.005	1.00	-239048.00
THR9	HG21	1.00	0.004	1.00	-1360443.00
THR9	H	1.00	0.001	1.00	-14033966.00
THR9	HG1	1.00	0.008	1.00	-70262.00
ASN10	H	1.00	0.009	1.00	-251052.00
ASN10	HB2	0.52	0.025	1.00	-238083.00

3.9.5 Detailed Probabilities of THR9HA:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN8	1.00	1.00
THR9	1.00	1.00
ASN10	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N8HA	1.00
T9HB	1.00
T9HG21	1.00
T9H	1.00
T9HG1	1.00
T9HA	1.00
N10H	1.00
N10HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN8	HA	1.00	0.005	1.00	0.11
THR9	HA	1.00	0.008	1.00	1.28
THR9	HB	1.00	0.018	1.00	0.56
THR9	HG21	1.00	0.007	1.00	0.34
THR9	H	1.00	0.011	1.00	-578376.00
ASN10	HA	1.00	0.026	1.00	0.21
ASN10	H	1.00	0.014	1.00	-1360954.00

3.9.6 Detailed Probabilities of THR9HB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
THR9	1.00	1.00
ASN10	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
T9HA	1.00
T9HG21	1.00
T9H	1.00
T9HG1	1.00
T9HB	1.00
N10H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR9	HA	1.00	0.024	1.00	0.28
THR9	HB	1.00	0.001	1.00	2.03
THR9	HG21	1.00	0.003	1.00	1.04
THR9	H	1.00	0.005	1.00	-239048.00
ASN10	H	1.00	0.000	1.00	-241708.00

3.9.7 Detailed Probabilities of THR9HG21:

Overall probability: 0.650

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
THR9	0.65	1.00

Expected NOESY Contacts

Proton	Expected probability
T9HA	1.00
T9HB	1.00
T9HG22	1.00
T9H	1.00
T9HG1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR9	HA	1.00	0.034	0.60	0.00
THR9	HB	1.00	0.004	1.00	1.06
THR9	HG21	1.00	0.103	0.00	0.00
THR9	H	1.00	0.004	1.00	-1360443.00

3.9.8 Detailed Probabilities of THR9H:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN8	1.00	1.00
THR9	0.50	1.00
ASN10	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N8H	1.00
N8HA	1.00
N8HB3	1.00
N8HB2	1.00
T9HA	1.00
T9HB	1.00
T9HG21	1.00
T9HG1	1.00
T9H	1.00
N10H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN8	HA	1.00	0.008	1.00	1.01
ASN8	HB2	1.00	0.005	1.00	0.05
ASN8	HB3	1.00	0.010	1.00	0.10
ASN8	H	1.00	0.008	1.00	-80144.00
ASN8	HD21	0.70	0.005	1.00	-215237.00
THR9	HA	1.00	0.046	0.00	0.00
THR9	HB	1.00	0.005	1.00	0.10
THR9	HG21	1.00	0.200	0.00	0.00
THR9	H	1.00	0.001	1.00	-14033966.00
ASN10	H	1.00	0.020	1.00	-80201.00
ASN10	HA	0.87	0.009	1.00	0.25

3.9.9 Detailed Probabilities of THR9HG1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
THR9	1.00	1.00
ASN10	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
T9HA	1.00
T9HB	1.00
T9HG21	1.00
T9H	1.00
N10H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR9	HA	1.00	0.008	1.00	0.59
THR9	HB	1.00	0.013	1.00	0.87
THR9	HG21	1.00	0.013	1.00	0.48
THR9	H	1.00	0.008	1.00	-70262.00
ASN10	H	0.97	0.012	1.00	-472079.00

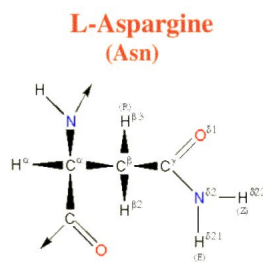
3.10 ASN(10)

Figure 10: Image from the BMRB

Residue probability: 0.824
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.601	175.315	1.862	0.000	0.000
CA 3.10.1	51.844	53.674	5.429	0.882	1.000
CB 3.10.2	39.316	38.785	5.449	0.714	1.000
N 3.10.3	123.266	118.907	6.480	0.835	1.000
ND2 3.10.4	111.462	112.932	14.355	1.000	1.000
HA 3.10.5	4.967	4.658	0.371	0.889	1.000
HB2 3.10.6	2.906	2.800	0.341	1.000	1.000
HB3 3.10.7	2.817	2.739	0.364	0.571	1.000
H 3.10.8	8.440	8.328	0.633	0.672	1.000
HD21 3.10.9	7.641	7.343	1.188	0.671	1.000
HD22 3.10.10	6.927	7.145	1.184	1.000	1.000

3.10.1 Detailed Probabilities of ASN10CA:

Overall probability: 0.882
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
THR9	1.00	1.00
ASN10	0.78	1.00
ASN11	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
T9HA	1.00
N10HB2	1.00
N10HB3	1.00
N10H	1.00
N10HD21	1.00
N10HD22	1.00
N10HA	1.00
N11HA	1.00
N11H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR9	HA	1.00	0.026	1.00	0.21
THR9	H	0.87	0.009	1.00	0.25
ASN10	HA	1.00	0.005	1.00	8.02
ASN10	HB2	1.00	0.004	1.00	1.13
ASN10	HB3	1.00	0.017	1.00	1.13
ASN10	H	1.00	0.033	0.70	0.00
ASN10	HD21	1.00	0.054	0.00	0.00
ASN10	HD22	1.00	0.000	1.00	0.27
ASN11	HA	1.00	0.020	1.00	0.21
ASN11	H	1.00	0.007	1.00	0.42
ASN11	HB2	0.51	0.003	1.00	0.19

3.10.2 Detailed Probabilities of ASN10CB:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN10	0.83	1.00
ASN11	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N10HA	1.00
N10HB3	1.00
N10H	1.00
N10HD21	1.00
N10HD22	1.00
N10HB2	1.00
N11H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN10	HA	1.00	0.006	1.00	0.83
ASN10	HB2	1.00	0.003	1.00	3.60
ASN10	HB3	1.00	0.086	0.00	0.00
ASN10	H	1.00	0.001	1.00	0.29
ASN10	HD21	1.00	0.003	1.00	0.32
ASN10	HD22	1.00	0.003	1.00	0.15
ASN11	H	1.00	0.073	0.00	0.00

3.10.3 Detailed Probabilities of ASN10N:

Overall probability: 0.835

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
THR9	1.00	1.00
ASN10	0.80	1.00
ASN11	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
T9HG1	0.97
T9HB	1.00
T9H	1.00
T9HA	1.00
N10HA	1.00
N10HB2	1.00
N10HB3	1.00
N10HD21	0.98
N10H	1.00
N11H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR9	HA	1.00	0.014	1.00	-1360954.00
THR9	HB	1.00	0.000	1.00	-241708.00
THR9	H	1.00	0.020	1.00	-80201.00
THR9	HG1	0.97	0.012	1.00	-472079.00
THR9	HG21	0.95	0.004	1.00	-313290.00
ASN10	HA	1.00	0.004	1.00	-414400.00
ASN10	HB2	1.00	0.000	1.00	-339821.00
ASN10	HB3	1.00	0.017	1.00	-380281.00
ASN10	H	1.00	0.003	1.00	-4670438.00
ASN10	HD21	0.98	0.383	0.02	0.00
ASN11	H	1.00	0.077	0.00	0.00
ASN11	HB2	0.60	0.002	1.00	-157298.00

3.10.4 Detailed Probabilities of ASN10ND2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN10	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N10HA	1.00
N10HB2	1.00
N10HB3	1.00
N10HD21	1.00
N10HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN10	HA	1.00	0.013	1.00	-111717.00
ASN10	HB2	1.00	0.008	1.00	-321330.00
ASN10	HB3	1.00	0.008	1.00	-389572.00
ASN10	HD21	1.00	0.000	1.00	-11257781.00
ASN10	HD22	1.00	0.002	1.00	-13846925.00

3.10.5 Detailed Probabilities of ASN10HA:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
THR9	1.00	1.00
ASN10	1.00	1.00
ASN11	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
T9HA	1.00
N10HB2	1.00
N10HB3	1.00
N10H	1.00
N10HD21	1.00
N10HD22	1.00
N10HA	1.00
N11HA	1.00
N11H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR9	HA	1.00	0.002	1.00	0.49
ASN10	HA	1.00	0.005	1.00	8.02
ASN10	HB2	1.00	0.006	1.00	0.83
ASN10	HB3	1.00	0.006	1.00	0.79
ASN10	H	1.00	0.004	1.00	-414400.00
ASN10	HD21	1.00	0.003	1.00	-160456.00
ASN10	HD22	1.00	0.013	1.00	-111717.00
ASN11	HA	1.00	0.387	0.00	0.00
ASN11	H	1.00	0.003	1.00	-403065.00

3.10.6 Detailed Probabilities of ASN10HB2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN10	1.00	1.00
ASN11	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N10HA	1.00
N10HB3	1.00
N10H	1.00
N10HD21	1.00
N10HD22	1.00
N10HB2	1.00
N11H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN10	HA	1.00	0.004	1.00	1.13
ASN10	HB2	1.00	0.003	1.00	3.60
ASN10	HB3	1.00	0.006	1.00	3.93
ASN10	H	1.00	0.000	1.00	-339821.00
ASN10	HD21	1.00	0.001	1.00	-480057.00
ASN10	HD22	1.00	0.008	1.00	-321330.00
ASN11	H	1.00	0.015	1.00	-133538.00

3.10.7 Detailed Probabilities of ASN10HB3:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN10	0.67	1.00
ASN11	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N10HA	1.00
N10HB2	1.00
N10H	1.00
N10HD21	1.00
N10HD22	1.00
N10HB3	1.00
N11H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN10	HA	1.00	0.017	1.00	1.13
ASN10	HB2	1.00	0.086	0.00	0.00
ASN10	HB3	1.00	0.095	0.00	0.00
ASN10	H	1.00	0.017	1.00	-380281.00
ASN10	HD21	1.00	0.013	1.00	-597526.00
ASN10	HD22	1.00	0.008	1.00	-389572.00
ASN11	H	1.00	0.073	0.00	0.00

3.10.8 Detailed Probabilities of ASN10H:

Overall probability: 0.672

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
THR9	0.67	1.00
ASN10	0.74	1.00
ASN11	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
T9HG1	0.97
T9HB	1.00
T9H	1.00
T9HA	1.00
N10HA	1.00
N10HB2	1.00
N10HB3	1.00
N10HD21	0.98
N10H	1.00
N11H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR9	HA	1.00	0.124	0.00	0.00
THR9	HB	1.00	0.001	1.00	0.26
THR9	H	1.00	0.009	1.00	-251052.00
ASN10	HA	1.00	0.033	0.70	0.00
ASN10	HB2	1.00	0.001	1.00	0.29
ASN10	HB3	1.00	0.002	1.00	0.27
ASN10	H	1.00	0.003	1.00	-4670438.00
ASN10	HD21	0.98	0.799	0.02	0.00
ASN11	H	1.00	0.069	0.00	0.00
ASN11	HB2	0.60	0.019	1.00	0.06

3.10.9 Detailed Probabilities of ASN10HD21:

Overall probability: 0.671

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN10	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
N10HA	1.00
N10HB2	1.00
N10HB3	1.00
N10H	0.98
N10HD22	1.00
N10HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN10	HA	1.00	0.054	0.00	0.00
ASN10	HB2	1.00	0.003	1.00	0.32
ASN10	HB3	1.00	0.000	1.00	0.39
ASN10	H	0.98	0.383	0.02	0.00
ASN10	HD21	1.00	0.000	1.00	-12698529.00
ASN10	HD22	1.00	0.000	1.00	-11257781.00

3.10.10 Detailed Probabilities of ASN10HD22:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN10	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N10HA	1.00
N10HB2	1.00
N10HB3	1.00
N10HD21	1.00
N10HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN10	HA	1.00	0.000	1.00	0.27
ASN10	HB2	1.00	0.003	1.00	0.15
ASN10	HB3	1.00	0.001	1.00	0.18
ASN10	HD21	1.00	0.003	1.00	-10419286.00
ASN10	HD22	1.00	0.002	1.00	-13846925.00

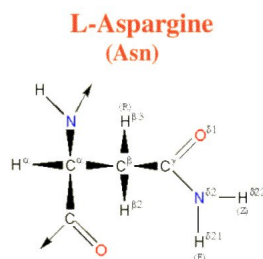
3.11 ASN(11)

Figure 11: Image from the BMRB

Residue probability: 0.834
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.333	175.315	1.862	0.000	0.000
CA 3.11.1	52.436	53.674	5.429	0.800	1.000
CB 3.11.2	38.349	38.785	5.449	0.714	1.000
N 3.11.3	120.920	118.907	6.480	0.833	1.000
ND2 3.11.4	114.074	112.932	14.355	1.000	1.000
HA 3.11.5	4.693	4.658	0.371	0.700	1.000
HB2 3.11.6	3.027	2.800	0.341	0.857	1.000
HB3 3.11.7	2.744	2.739	0.364	0.714	1.000
H 3.11.8	8.366	8.328	0.633	0.718	1.000
HD21 3.11.9	7.334	7.343	1.188	1.000	1.000
HD22 3.11.10	7.335	7.145	1.184	1.000	1.000

3.11.1 Detailed Probabilities of ASN11CA:

Overall probability: 0.800
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN10	0.00	1.00
ASN11	0.83	1.00
ASP12	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N10HA	1.00
N11HB2	1.00
N11HB3	1.00
N11H	1.00
N11HD21	1.00
N11HD22	1.00
N11HA	1.00
D12HA	1.00
D12H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN10	HA	1.00	0.387	0.00	0.00
ASN11	HA	1.00	0.394	0.00	0.00
ASN11	HB2	1.00	0.010	1.00	1.03
ASN11	HB3	1.00	0.017	1.00	0.67
ASN11	H	1.00	0.025	1.00	0.33
ASN11	HD21	1.00	0.023	1.00	0.26
ASN11	HD22	1.00	0.024	1.00	0.26
ASP12	HA	1.00	0.026	1.00	0.19
ASP12	H	1.00	0.006	1.00	1.66
ASP12	HB2	0.53	0.027	1.00	0.25

3.11.2 Detailed Probabilities of ASN11CB:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN11	0.67	1.00
ASP12	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N11HA	1.00
N11HB2	1.00
N11H	1.00
N11HD21	1.00
N11HD22	1.00
N11HB3	1.00
D12H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN11	HA	1.00	1.496	0.00	0.00
ASN11	HB2	1.00	0.004	1.00	1.14
ASN11	HB3	1.00	0.279	0.00	0.00
ASN11	H	1.00	0.005	1.00	0.43
ASN11	HD21	1.00	0.009	1.00	0.38
ASN11	HD22	1.00	0.008	1.00	0.38
ASP12	H	1.00	0.005	1.00	0.10

3.11.3 Detailed Probabilities of ASN11N:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN10	0.50	1.00
ASN11	1.00	1.00
ASP12	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N10HA	1.00
N10HB2	1.00
N10H	1.00
N10HB3	1.00
N11HA	1.00
N11HB2	1.00
N11HB3	1.00
N11HD21	0.98
N11H	1.00
D12H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN10	HA	1.00	0.003	1.00	-403065.00
ASN10	HB2	1.00	0.015	1.00	-133538.00
ASN10	HB3	1.00	0.073	0.00	0.00
ASN10	H	1.00	0.069	0.00	0.00
ASN11	HA	1.00	0.008	1.00	-568209.00
ASN11	HB2	1.00	0.001	1.00	-973176.00
ASN11	HB3	1.00	0.000	1.00	-879800.00
ASN11	H	1.00	0.005	1.00	-5990068.00
ASN11	HD21	0.98	0.006	1.00	-173454.00
ASN11	HD22	0.63	0.005	1.00	-173454.00
ASP12	H	1.00	0.003	1.00	-192466.00
ASP12	HA	0.86	0.010	1.00	-103502.00

3.11.4 Detailed Probabilities of ASN11ND2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN11	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N11HA	1.00
N11HB2	1.00
N11HB3	1.00
N11H	0.98
N11HD22	1.00
N11HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN11	HA	1.00	0.008	1.00	-112595.00
ASN11	HB2	1.00	0.000	1.00	-276602.00
ASN11	HB3	1.00	0.003	1.00	-405664.00
ASN11	H	0.98	0.020	1.00	-101435.00
ASN11	HD21	1.00	0.006	1.00	-9261102.00
ASN11	HD22	1.00	0.005	1.00	-9261102.00

3.11.5 Detailed Probabilities of ASN11HA:

Overall probability: 0.700

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN10	1.00	1.00
ASN11	0.50	1.00
ASP12	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N10HA	1.00
N11HB2	1.00
N11HB3	1.00
N11H	1.00
N11HD21	1.00
N11HD22	1.00
N11HA	1.00
D12HA	1.00
D12H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN10	HA	1.00	0.020	1.00	0.21
ASN11	HA	1.00	0.394	0.00	0.00
ASN11	HB2	1.00	0.184	0.00	0.00
ASN11	HB3	1.00	1.496	0.00	0.00
ASN11	H	1.00	0.008	1.00	-568209.00
ASN11	HD21	1.00	0.008	1.00	-112595.00
ASN11	HD22	1.00	0.008	1.00	-112595.00
ASP12	HA	1.00	0.008	1.00	0.09
ASP12	H	1.00	0.002	1.00	-2251462.00
ASP12	HB2	0.53	0.009	1.00	0.47

3.11.6 Detailed Probabilities of ASN11HB2:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN11	0.83	1.00
ASP12	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N11HA	1.00
N11HB3	1.00
N11H	1.00
N11HD21	1.00
N11HD22	1.00
N11HB2	1.00
D12H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN11	HA	1.00	0.010	1.00	1.03
ASN11	HB2	1.00	0.279	0.00	0.00
ASN11	HB3	1.00	0.004	1.00	1.14
ASN11	H	1.00	0.001	1.00	-973176.00
ASN11	HD21	1.00	0.000	1.00	-276602.00
ASN11	HD22	1.00	0.000	1.00	-276602.00
ASP12	H	1.00	0.003	1.00	-94668.00

3.11.7 Detailed Probabilities of ASN11HB3:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN11	0.83	1.00
ASP12	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N11HA	1.00
N11HB2	1.00
N11H	1.00
N11HD21	1.00
N11HD22	1.00
N11HB3	1.00
D12H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN11	HA	1.00	0.017	1.00	0.67
ASN11	HB2	1.00	0.004	1.00	1.10
ASN11	HB3	1.00	0.279	0.00	0.00
ASN11	H	1.00	0.000	1.00	-879800.00
ASN11	HD21	1.00	0.003	1.00	-405664.00
ASN11	HD22	1.00	0.003	1.00	-405664.00
ASP12	H	1.00	0.098	0.00	0.00

3.11.8 Detailed Probabilities of ASN11H:**Overall probability:** 0.718**Overall confidence:** 1.000**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASN10	0.25	1.00
ASN11	1.00	1.00
ASP12	0.90	1.00

Expected NOESY Contacts

Proton	Expected probability
N10HA	1.00
N10HB2	1.00
N10H	1.00
N10HB3	1.00
N11HA	1.00
N11HB2	1.00
N11HB3	1.00
N11HD21	0.98
N11H	1.00
D12H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN10	HA	1.00	0.007	1.00	0.42
ASN10	HB2	1.00	0.073	0.00	0.00
ASN10	HB3	1.00	0.076	0.00	0.00
ASN10	H	1.00	0.077	0.00	0.00
ASN11	HA	1.00	0.025	1.00	0.33
ASN11	HB2	1.00	0.007	1.00	0.38
ASN11	HB3	1.00	0.005	1.00	0.43
ASN11	H	1.00	0.005	1.00	-5990068.00
ASN11	HD21	0.98	0.020	1.00	-101435.00
ASN11	HD22	0.63	0.020	1.00	-101435.00
ASP12	H	1.00	0.031	0.90	0.00

3.11.9 Detailed Probabilities of ASN11HD21:**Overall probability:** 1.000**Overall confidence:** 1.000**Inter- and intra-residue probability**

Residue	Probability	Confidence
ASN11	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N11HA	1.00
N11HB2	1.00
N11HB3	1.00
N11H	0.98
N11HD22	1.00
N11HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN11	HA	1.00	0.023	1.00	0.26
ASN11	HB2	1.00	0.006	1.00	0.25
ASN11	HB3	1.00	0.009	1.00	0.38
ASN11	H	0.98	0.006	1.00	-173454.00
ASN11	HD21	1.00	0.006	1.00	-9261102.00
ASN11	HD22	1.00	0.006	1.00	-9261102.00

3.11.10 Detailed Probabilities of ASN11HD22:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN11	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N11HA	1.00
N11HB2	1.00
N11HB3	1.00
N11HD21	1.00
N11HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN11	HA	1.00	0.024	1.00	0.26
ASN11	HB2	1.00	0.005	1.00	0.25
ASN11	HB3	1.00	0.008	1.00	0.38
ASN11	HD21	1.00	0.005	1.00	-9261102.00
ASN11	HD22	1.00	0.005	1.00	-9261102.00
ASN11	H	0.63	0.005	1.00	-173454.00

3.12 ASP(12)

Figure 12: Image from the BMRB

Residue probability: 0.929

Residue probability confidence: 0.886

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.089	176.463	2.348	0.000	0.000
CA 3.12.1	57.608	54.786	4.266	0.967	0.857
CB 3.12.2	41.161	40.949	3.070	1.000	0.800
N 3.12.3	126.315	120.550	5.690	0.878	1.000
HD2	NA	—	—	0.000	0.000
HA 3.12.4	4.273	4.587	0.329	0.857	0.857
HB 3.12.5	2.642	2.708	0.282	1.000	0.800
H 3.12.6	8.586	8.304	1.027	0.875	1.000

3.12.1 Detailed Probabilities of ASP12CA:

Overall probability: 0.967

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN11	1.00	1.00
ASP12	1.00	0.75
GLU13	0.90	1.00

Expected NOESY Contacts

Proton	Expected probability
N11HA	1.00
D12HD2	1.00
D12HB2	1.00
D12H	1.00
D12HA	1.00
E13H	1.00
E13HA	1.00

NOESY contacts detailed probability

3.12 ASP(12)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN11	HA	1.00	0.008	1.00	0.09
ASP12	HA	1.00	0.009	1.00	12.17
ASP12	HB2	1.00	0.002	1.00	1.35
ASP12	H	1.00	0.007	1.00	0.49
GLU13	HA	1.00	0.012	1.00	0.10
GLU13	H	1.00	0.032	0.80	0.00

3.12.2 Detailed Probabilities of ASP12CB:

Overall probability: 1.000

Overall confidence: 0.800

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP12	1.00	0.75
GLU13	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D12HD2	1.00
D12HA	1.00
D12HB3	1.00
D12H	1.00
E13H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP12	HA	1.00	0.008	1.00	1.08
ASP12	HB2	1.00	0.007	1.00	25.87
ASP12	H	1.00	0.007	1.00	0.84
GLU13	H	1.00	0.006	1.00	0.42

3.12.3 Detailed Probabilities of ASP12N:

Overall probability: 0.878

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN11	0.72	1.00
ASP12	1.00	1.00
GLU13	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N11HB3	1.00
N11HB2	1.00
N11HA	1.00
N11H	1.00
D12HA	1.00
D12HB2	1.00
D12H	1.00
E13H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN11	HA	1.00	0.002	1.00	-2251462.00
ASN11	HB2	1.00	0.003	1.00	-94668.00
ASN11	HB3	1.00	0.098	0.00	0.00
ASN11	H	1.00	0.031	0.90	0.00
ASP12	HA	1.00	0.005	1.00	-862589.00
ASP12	HB2	1.00	0.004	1.00	-1883332.00
ASP12	H	1.00	0.005	1.00	-7359728.00
GLU13	H	1.00	0.005	1.00	-815091.00
GLU13	HA	0.86	0.000	1.00	-99629.00

3.12.4 Detailed Probabilities of ASP12HA:

Overall probability: 0.857

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN11	1.00	1.00
ASP12	1.00	0.75
GLU13	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
N11HA	1.00
D12HD2	1.00
D12HB2	1.00
D12H	1.00
D12HA	1.00
E13H	1.00
E13HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN11	HA	1.00	0.026	1.00	0.19
ASN11	H	0.86	0.010	1.00	-103502.00
ASP12	HA	1.00	0.009	1.00	12.17
ASP12	HB2	1.00	0.008	1.00	1.08
ASP12	H	1.00	0.005	1.00	-862589.00
GLU13	HA	1.00	0.231	0.00	0.00
GLU13	H	1.00	0.008	1.00	-358055.00

3.12.5 Detailed Probabilities of ASP12HB2:

Overall probability: 1.000

Overall confidence: 0.800

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP12	1.00	0.75
GLU13	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D12HD2	1.00
D12HA	1.00
D12HB3	1.00
D12H	1.00
E13H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP12	HA	1.00	0.002	1.00	1.35
ASP12	HB2	1.00	0.007	1.00	25.87
ASP12	H	1.00	0.004	1.00	-1883332.00
GLU13	H	1.00	0.002	1.00	-809987.00
GLU13	HA	0.84	0.001	1.00	0.09

3.12.6 Detailed Probabilities of ASP12H:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN11	0.75	1.00
ASP12	1.00	1.00
GLU13	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N11HB3	1.00
N11HB2	1.00
N11HA	1.00
N11H	1.00
D12HA	1.00
D12HB2	1.00
D12H	1.00
E13H	1.00

NOESY contacts detailed probability					
Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN11	HA	1.00	0.006	1.00	1.66
ASN11	HB2	1.00	0.127	0.00	0.00
ASN11	HB3	1.00	0.005	1.00	0.10
ASN11	H	1.00	0.003	1.00	-192466.00
ASP12	HA	1.00	0.007	1.00	0.49
ASP12	HB2	1.00	0.007	1.00	0.84
ASP12	H	1.00	0.005	1.00	-7359728.00
GLU13	H	1.00	0.006	1.00	-642560.00

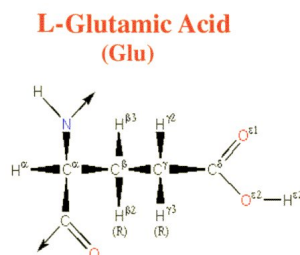
3.13 GLU(13)

Figure 13: Image from the BMRB

Residue probability: 0.731

Residue probability confidence: 0.925

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.893	176.942	2.547	0.000	0.000
CA 3.13.1	59.006	57.442	3.837	0.600	1.000
CB 3.13.2	28.709	30.185	4.018	0.571	0.875
CG 3.13.3	36.010	36.085	1.533	0.857	0.875
N 3.13.4	119.325	120.574	4.837	1.000	1.000
HA 3.13.5	4.026	4.245	0.429	0.820	1.000
HB2 3.13.6	2.064	2.021	0.233	0.714	0.875
HB3 3.13.7	2.160	1.994	0.244	0.571	0.875
HG2 3.13.8	2.361	2.258	0.226	0.571	0.875
HG3 3.13.9	2.310	2.233	0.232	0.714	0.875
H 3.13.10	8.289	8.332	0.601	0.891	1.000
HE2	NA	—	—	0.000	0.000

3.13.1 Detailed Probabilities of GLU13CA:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP12	0.50	1.00
GLU13	0.83	1.00
LEU14	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D12HA	1.00
E13HB2	1.00
E13HB3	1.00
E13HG2	1.00
E13HG3	1.00
E13H	1.00
E13HA	1.00
L14H	1.00
L14HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP12	HA	1.00	0.231	0.00	0.00
ASP12	HB2	0.54	0.001	1.00	0.09
GLU13	HA	1.00	0.016	1.00	41.95
GLU13	HB2	1.00	0.014	1.00	5.05
GLU13	HB3	1.00	0.005	1.00	2.61
GLU13	HG2	1.00	0.079	0.00	0.00
GLU13	HG3	1.00	0.028	1.00	2.14
GLU13	H	1.00	0.010	1.00	0.79
LEU14	HA	1.00	0.057	0.00	0.00
LEU14	H	1.00	0.051	0.00	0.00

3.13.2 Detailed Probabilities of GLU13CB:

Overall probability: 0.571

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU13	0.50	0.86
LEU14	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E13HA	1.00
E13HB3	1.00
E13HG2	1.00
E13HG3	1.00
E13H	1.00
E13HE2	1.00
E13HB2	1.00
L14H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU13	HA	1.00	0.010	1.00	2.70
GLU13	HB2	1.00	0.271	0.00	0.00
GLU13	HB3	1.00	0.175	0.00	0.00
GLU13	HG2	1.00	0.026	1.00	4.32
GLU13	HG3	1.00	0.025	1.00	4.32
GLU13	H	1.00	0.193	0.00	0.00
LEU14	H	1.00	0.013	1.00	0.57

3.13.3 Detailed Probabilities of GLU13CG:

Overall probability: 0.857

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU13	0.83	0.86
LEU14	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E13HA	1.00
E13HB2	1.00
E13HB3	1.00
E13HG3	1.00
E13H	1.00
E13HE2	1.00
E13HG2	1.00
L14H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU13	HA	1.00	0.010	1.00	1.15
GLU13	HB2	1.00	0.027	1.00	3.11
GLU13	HB3	1.00	0.029	1.00	5.21
GLU13	HG2	1.00	0.030	1.00	30.23
GLU13	HG3	1.00	0.365	0.00	0.00
GLU13	H	1.00	0.005	1.00	0.70
LEU14	H	0.98	0.013	1.00	0.19

3.13.4 Detailed Probabilities of GLU13N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP12	1.00	1.00
GLU13	1.00	1.00
LEU14	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D12H	1.00
D12HA	1.00
D12HB3	1.00
E13HA	1.00
E13HB2	1.00
E13HB3	1.00
E13HG2	1.00
E13HG3	1.00
E13H	1.00
L14H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP12	HA	1.00	0.008	1.00	-358055.00
ASP12	HB2	1.00	0.002	1.00	-809987.00
ASP12	H	1.00	0.006	1.00	-642560.00
GLU13	HA	1.00	0.002	1.00	-973370.00
GLU13	HB2	1.00	0.007	1.00	-832025.00
GLU13	HB3	1.00	0.004	1.00	-1278868.00
GLU13	HG2	1.00	0.030	1.00	0.00
GLU13	HG3	1.00	0.021	1.00	-828480.00
GLU13	H	1.00	0.005	1.00	-9951911.00
LEU14	H	1.00	0.006	1.00	-1152303.00

3.13.5 Detailed Probabilities of GLU13HA:

Overall probability: 0.820

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP12	1.00	1.00
GLU13	0.83	1.00
LEU14	0.60	1.00

Expected NOESY Contacts

Proton	Expected probability
D12HA	1.00
E13HB2	1.00
E13HB3	1.00
E13HG2	1.00
E13HG3	1.00
E13H	1.00
E13HA	1.00
L14H	1.00
L14HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP12	HA	1.00	0.012	1.00	0.10
ASP12	H	0.86	0.000	1.00	-99629.00
GLU13	HA	1.00	0.016	1.00	41.95
GLU13	HB2	1.00	0.010	1.00	2.70
GLU13	HB3	1.00	1.383	0.00	0.00
GLU13	HG2	1.00	0.010	1.00	1.15
GLU13	HG3	1.00	0.011	1.00	2.08
GLU13	H	1.00	0.002	1.00	-973370.00
LEU14	HA	1.00	0.038	0.20	0.00
LEU14	H	1.00	0.025	1.00	-796320.00

3.13.6 Detailed Probabilities of GLU13HB2:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU13	0.67	0.86
LEU14	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E13HA	1.00
E13HB3	1.00
E13HG2	1.00
E13HG3	1.00
E13H	1.00
E13HE2	1.00
E13HB2	1.00
L14H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU13	HA	1.00	0.014	1.00	5.05
GLU13	HB2	1.00	0.271	0.00	0.00
GLU13	HB3	1.00	0.579	0.00	0.00
GLU13	HG2	1.00	0.027	1.00	3.11
GLU13	HG3	1.00	0.016	1.00	8.87
GLU13	H	1.00	0.007	1.00	-832025.00
LEU14	H	1.00	0.011	1.00	-450110.00

3.13.7 Detailed Probabilities of GLU13HB3:

Overall probability: 0.571

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU13	0.50	0.86
LEU14	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E13HA	1.00
E13HB2	1.00
E13HG2	1.00
E13HG3	1.00
E13H	1.00
E13HE2	1.00
E13HB3	1.00
L14H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU13	HA	1.00	0.005	1.00	2.61
GLU13	HB2	1.00	0.175	0.00	0.00
GLU13	HB3	1.00	0.483	0.00	0.00
GLU13	HG2	1.00	0.029	1.00	5.21
GLU13	HG3	1.00	0.080	0.00	0.00
GLU13	H	1.00	0.004	1.00	-1278868.00
LEU14	H	1.00	0.004	1.00	-558737.00

3.13.8 Detailed Probabilities of GLU13HG2:

Overall probability: 0.571

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU13	0.50	0.86
LEU14	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E13HA	1.00
E13HB2	1.00
E13HB3	1.00
E13HG3	1.00
E13H	1.00
E13HE2	1.00
E13HG2	1.00
L14H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU13	HA	1.00	0.079	0.00	0.00
GLU13	HB2	1.00	0.026	1.00	4.32
GLU13	HB3	1.00	0.282	0.00	0.00
GLU13	HG2	1.00	0.030	1.00	30.23
GLU13	HG3	1.00	0.281	0.00	0.00
GLU13	H	1.00	0.030	1.00	0.00
LEU14	H	0.98	0.021	1.00	-216409.00

3.13.9 Detailed Probabilities of GLU13HG3:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU13	0.67	0.86
LEU14	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E13HA	1.00
E13HB2	1.00
E13HB3	1.00
E13HG2	1.00
E13H	1.00
E13HE2	1.00
E13HG3	1.00
L14H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU13	HA	1.00	0.028	1.00	2.14
GLU13	HB2	1.00	0.025	1.00	4.32
GLU13	HB3	1.00	0.333	0.00	0.00
GLU13	HG2	1.00	0.365	0.00	0.00
GLU13	HG3	1.00	0.014	1.00	100.68
GLU13	H	1.00	0.021	1.00	-828480.00
LEU14	H	0.97	0.030	1.00	-216409.00

3.13.10 Detailed Probabilities of GLU13H:

Overall probability: 0.891

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP12	0.93	1.00
GLU13	0.83	1.00
LEU14	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D12H	1.00
D12HA	1.00
D12HB3	1.00
E13HA	1.00
E13HB2	1.00
E13HB3	1.00
E13HG2	1.00
E13HG3	1.00
E13H	1.00
L14H	1.00

NOESY contacts detailed probability

3.13 GLU(13)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP12	HA	1.00	0.032	0.80	0.00
ASP12	HB2	1.00	0.006	1.00	0.42
ASP12	H	1.00	0.005	1.00	-815091.00
GLU13	HA	1.00	0.010	1.00	0.79
GLU13	HB2	1.00	0.193	0.00	0.00
GLU13	HB3	1.00	0.003	1.00	0.94
GLU13	HG2	1.00	0.005	1.00	0.70
GLU13	HG3	1.00	0.005	1.00	0.70
GLU13	H	1.00	0.005	1.00	-9951911.00
LEU14	H	1.00	0.010	1.00	-1398261.00
LEU14	HA	0.93	0.001	1.00	0.13

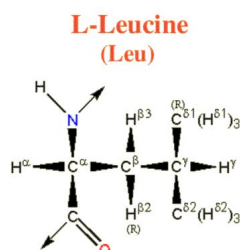
3.14 LEU(14)

Figure 14: Image from the BMRB

Residue probability: 0.685

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.309	177.056	1.929	0.000	0.000
CA 3.14.1	57.261	55.735	3.802	0.767	1.000
CB 3.14.2	40.105	42.389	3.750	0.750	1.000
CG 3.14.3	27.050	26.892	3.086	0.875	1.000
CD1 3.14.4	22.485	24.837	3.657	0.714	1.000
CD2 3.14.5	24.529	24.201	3.117	0.001	1.000
N 3.14.6	121.683	121.785	4.943	0.938	1.000
HA 3.14.7	3.985	4.315	0.840	0.601	1.000
HB2 3.14.8	1.823	1.601	0.373	0.667	1.000
HB3 3.14.9	1.498	1.508	0.398	0.750	1.000
HG 3.14.10	1.378	1.510	0.340	0.627	1.000
HD1 3.14.11	0.859	0.739	0.294	0.714	1.000
HD2 3.14.12	0.763	0.727	0.421	0.571	1.000
H 3.14.13	7.577	8.237	0.647	0.933	1.000

3.14.1 Detailed Probabilities of LEU14CA:

Overall probability: 0.767

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU13	0.60	1.00
LEU14	1.00	1.00
ILE15	0.33	1.00

Expected NOESY Contacts

Proton	Expected probability
E13HA	1.00
L14HB2	1.00
L14HB3	1.00
L14HG	1.00
L14HD11	0.99
L14HD21	0.99
L14H	1.00
L14HA	1.00
I15H	1.00
I15HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU13	HA	1.00	0.038	0.20	0.00
GLU13	H	0.93	0.001	1.00	0.13
LEU14	HA	1.00	0.003	1.00	4.86
LEU14	HB2	1.00	0.008	1.00	0.38
LEU14	HB3	1.00	0.013	1.00	0.79
LEU14	HG	1.00	0.020	1.00	0.34
LEU14	HD11	0.99	0.006	1.00	1.48
LEU14	HD21	0.99	0.006	1.00	0.42
LEU14	H	1.00	0.005	1.00	0.64
ILE15	HA	1.00	0.356	0.00	0.00
ILE15	H	1.00	0.050	0.00	0.00
ILE15	HG13	0.63	0.006	1.00	0.15

3.14.2 Detailed Probabilities of LEU14CB:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU14	0.86	1.00
ILE15	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L14HA	1.00
L14HB2	1.00
L14HG	1.00
L14HD11	1.00
L14HD21	1.00
L14H	1.00
L14HB3	1.00
I15H	1.00

NOESY contacts detailed probability

3.14 LEU(14)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU14	HA	1.00	0.003	1.00	0.25
LEU14	HB2	1.00	0.004	1.00	0.63
LEU14	HB3	1.00	0.006	1.00	0.83
LEU14	HG	1.00	0.010	1.00	0.40
LEU14	HD11	1.00	0.097	0.00	0.00
LEU14	HD21	1.00	0.001	1.00	0.57
LEU14	H	1.00	0.000	1.00	0.33
ILE15	H	1.00	0.661	0.00	0.00

3.14.3 Detailed Probabilities of LEU14CG:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU14	0.86	1.00
ILE15	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L14HA	1.00
L14HB2	1.00
L14HB3	1.00
L14HD11	1.00
L14HD21	1.00
L14H	1.00
L14HG	1.00
I15H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU14	HA	1.00	0.007	1.00	0.16
LEU14	HB2	1.00	0.009	1.00	0.44
LEU14	HB3	1.00	0.124	0.00	0.00
LEU14	HG	1.00	0.004	1.00	3.85
LEU14	HD11	1.00	0.002	1.00	1.15
LEU14	HD21	1.00	0.005	1.00	1.84
LEU14	H	1.00	0.002	1.00	0.10
ILE15	H	0.99	0.010	1.00	0.07

3.14.4 Detailed Probabilities of LEU14CD1:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU14	0.71	1.00

Expected NOESY Contacts

Proton	Expected probability
L14HA	0.99
L14HB2	1.00
L14HB3	1.00
L14HG	1.00
L14HD12	1.00
L14HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU14	HA	0.99	0.004	1.00	1.52
LEU14	HB2	1.00	0.192	0.00	0.00
LEU14	HB3	1.00	0.011	1.00	1.27
LEU14	HG	1.00	0.030	1.00	0.00
LEU14	HD11	1.00	0.020	1.00	78.79
LEU14	HD21	1.00	0.116	0.00	0.00
LEU14	H	0.86	0.017	1.00	0.40

3.14.5 Detailed Probabilities of LEU14CD2:

Overall probability: 0.001

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU14	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L14HA	0.99
L14HB2	1.00
L14HB3	1.00
L14HG	1.00
L14HD11	1.00
L14HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU14	HA	0.99	0.068	0.01	0.00
LEU14	HB2	1.00	0.431	0.00	0.00
LEU14	HB3	1.00	0.756	0.00	0.00
LEU14	HG	1.00	0.876	0.00	0.00
LEU14	HD11	1.00	0.617	0.00	0.00
LEU14	HD21	1.00	0.521	0.00	0.00

3.14.6 Detailed Probabilities of LEU14N:

Overall probability: 0.938

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU13	1.00	1.00
LEU14	1.00	1.00
ILE15	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
E13HB2	1.00
E13HG2	0.98
E13HG3	0.97
E13HB3	1.00
E13H	1.00
E13HA	1.00
L14HA	1.00
L14HB2	1.00
L14HB3	1.00
L14HG	1.00
L14H	1.00
I15H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU13	HA	1.00	0.025	1.00	-796320.00
GLU13	HB2	1.00	0.011	1.00	-450110.00
GLU13	HB3	1.00	0.004	1.00	-558737.00
GLU13	HG2	0.98	0.021	1.00	-216409.00
GLU13	HG3	0.97	0.030	1.00	-216409.00
GLU13	H	1.00	0.010	1.00	-1398261.00
LEU14	HA	1.00	0.016	1.00	-796320.00
LEU14	HB2	1.00	0.003	1.00	-907200.00
LEU14	HB3	1.00	0.004	1.00	-901843.00
LEU14	HG	1.00	0.005	1.00	-358289.00
LEU14	H	1.00	0.003	1.00	-6612363.00
LEU14	HD11	0.88	0.005	1.00	-511759.00
LEU14	HD21	0.87	0.002	1.00	-502682.00
ILE15	H	1.00	0.041	0.00	0.00
ILE15	HB	0.52	0.007	1.00	-187377.00
ILE15	HG13	0.58	0.012	1.00	-111429.00

3.14.7 Detailed Probabilities of LEU14HA:

Overall probability: 0.601

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU13	0.00	1.00
LEU14	0.86	1.00
ILE15	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E13HA	1.00
L14HB2	1.00
L14HB3	1.00
L14HG	1.00
L14HD11	0.99
L14HD21	0.99
L14H	1.00
L14HA	1.00
I15H	1.00
I15HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU13	HA	1.00	0.057	0.00	0.00
LEU14	HA	1.00	0.003	1.00	4.86
LEU14	HB2	1.00	0.011	1.00	0.17
LEU14	HB3	1.00	0.003	1.00	0.25
LEU14	HG	1.00	0.007	1.00	0.16
LEU14	HD11	0.99	0.004	1.00	1.52
LEU14	HD21	0.99	0.068	0.01	0.00
LEU14	H	1.00	0.016	1.00	-796320.00
ILE15	HA	1.00	0.609	0.00	0.00
ILE15	H	1.00	0.069	0.00	0.00

3.14.8 Detailed Probabilities of LEU14HB2:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU14	0.57	1.00
ILE15	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L14HA	1.00
L14HB3	1.00
L14HG	1.00
L14HD11	1.00
L14HD21	1.00
L14H	1.00
L14HB2	1.00
I15H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU14	HA	1.00	0.008	1.00	0.38
LEU14	HB2	1.00	0.316	0.00	0.00
LEU14	HB3	1.00	0.004	1.00	0.63
LEU14	HG	1.00	0.009	1.00	0.44
LEU14	HD11	1.00	0.192	0.00	0.00
LEU14	HD21	1.00	0.431	0.00	0.00
LEU14	H	1.00	0.003	1.00	-907200.00
ILE15	H	1.00	0.005	1.00	-466690.00
ILE15	HA	0.60	0.001	1.00	0.62

3.14.9 Detailed Probabilities of LEU14HB3:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU14	0.71	1.00
ILE15	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L14HA	1.00
L14HB2	1.00
L14HG	1.00
L14HD11	1.00
L14HD21	1.00
L14H	1.00
L14HB3	1.00
I15H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU14	HA	1.00	0.013	1.00	0.79
LEU14	HB2	1.00	0.009	1.00	0.75
LEU14	HB3	1.00	0.006	1.00	0.83
LEU14	HG	1.00	0.124	0.00	0.00
LEU14	HD11	1.00	0.011	1.00	1.27
LEU14	HD21	1.00	0.756	0.00	0.00
LEU14	H	1.00	0.004	1.00	-901843.00
ILE15	H	1.00	0.026	1.00	-1002986.00

3.14.10 Detailed Probabilities of LEU14HG:

Overall probability: 0.627

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU14	0.71	1.00
ILE15	0.01	1.00

Expected NOESY Contacts

Proton	Expected probability
L14HA	1.00
L14HB2	1.00
L14HB3	1.00
L14HD11	1.00
L14HD21	1.00
L14H	1.00
L14HG	1.00
I15H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU14	HA	1.00	0.020	1.00	0.34
LEU14	HB2	1.00	0.129	0.00	0.00
LEU14	HB3	1.00	0.010	1.00	0.40
LEU14	HG	1.00	0.004	1.00	3.85
LEU14	HD11	1.00	0.030	1.00	0.00
LEU14	HD21	1.00	0.876	0.00	0.00
LEU14	H	1.00	0.005	1.00	-358289.00
ILE15	H	0.99	0.094	0.01	0.00

3.14.11 Detailed Probabilities of LEU14HD11:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU14	0.71	1.00

Expected NOESY Contacts

Proton	Expected probability
L14HA	0.99
L14HB2	1.00
L14HB3	1.00
L14HG	1.00
L14HD12	1.00
L14HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU14	HA	0.99	0.006	1.00	1.48
LEU14	HB2	1.00	0.008	1.00	0.40
LEU14	HB3	1.00	0.097	0.00	0.00
LEU14	HG	1.00	0.002	1.00	1.15
LEU14	HD11	1.00	0.020	1.00	78.79
LEU14	HD21	1.00	0.617	0.00	0.00
LEU14	H	0.86	0.005	1.00	-511759.00

3.14.12 Detailed Probabilities of LEU14HD21:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU14	0.57	1.00

Expected NOESY Contacts

Proton	Expected probability
L14HA	0.99
L14HB2	1.00
L14HB3	1.00
L14HG	1.00
L14HD11	1.00
L14HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU14	HA	0.99	0.006	1.00	0.42
LEU14	HB2	1.00	0.104	0.00	0.00
LEU14	HB3	1.00	0.001	1.00	0.57
LEU14	HG	1.00	0.005	1.00	1.84
LEU14	HD11	1.00	0.116	0.00	0.00
LEU14	HD21	1.00	0.521	0.00	0.00
LEU14	H	0.85	0.002	1.00	-502682.00

3.14.13 Detailed Probabilities of LEU14H:

Overall probability: 0.933

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU13	0.83	1.00
LEU14	1.00	1.00
ILE15	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E13HB2	1.00
E13HG2	0.98
E13HG3	0.97
E13HB3	1.00
E13H	1.00
E13HA	1.00
L14HA	1.00
L14HB2	1.00
L14HB3	1.00
L14HG	1.00
L14H	1.00
I15H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU13	HA	1.00	0.051	0.00	0.00
GLU13	HB2	1.00	0.013	1.00	0.57
GLU13	HB3	1.00	0.003	1.00	0.38
GLU13	HG2	0.98	0.013	1.00	0.19
GLU13	HG3	0.97	0.013	1.00	0.19
GLU13	H	1.00	0.006	1.00	-1152303.00
LEU14	HA	1.00	0.005	1.00	0.64
LEU14	HB2	1.00	0.000	1.00	0.31
LEU14	HB3	1.00	0.000	1.00	0.33
LEU14	HG	1.00	0.002	1.00	0.10
LEU14	H	1.00	0.003	1.00	-6612363.00
LEU14	HD11	0.88	0.017	1.00	0.40
ILE15	H	1.00	0.011	1.00	-1320468.00
ILE15	HA	0.93	0.024	1.00	0.24
ILE15	HB	0.52	0.028	1.00	0.42

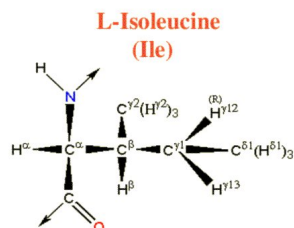


Figure 15: Image from the BMRB

Residue probability: 0.744
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	177.138	175.926	2.710	0.000	0.000
CA 3.15.1	66.590	61.717	4.152	0.833	1.000
CB 3.15.2	37.424	38.702	3.945	0.778	1.000
CG1 3.15.3	30.331	27.785	2.037	1.000	1.000
CG2 3.15.4	17.078	17.574	1.928	0.556	1.000
CD1 3.15.5	13.066	13.545	3.646	0.575	1.000
N 3.15.6	119.483	121.467	6.098	0.868	1.000
HA 3.15.7	3.219	4.185	1.403	0.703	1.000
HB 3.15.8	1.915	1.776	0.310	0.778	1.000
HG12 3.15.9	1.726	1.271	0.411	0.628	1.000
HG13 3.15.10	0.636	1.186	0.426	0.714	1.000
HG2 3.15.11	0.847	0.762	0.283	0.875	1.000
HD1 3.15.12	0.764	0.668	0.293	0.572	1.000
H 3.15.13	8.238	8.301	0.685	0.786	1.000

3.15.1 Detailed Probabilities of ILE15CA:

Overall probability: 0.833
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU14	0.67	1.00
ILE15	1.00	1.00
LYS16	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
L14HA	1.00
I15HB	1.00
I15HG12	1.00
I15HG13	1.00
I15HG21	1.00
I15HD11	0.97
I15H	1.00
I15HA	1.00
K16H	1.00
K16HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU14	HA	1.00	0.609	0.00	0.00
LEU14	HB2	0.60	0.001	1.00	0.62
LEU14	H	0.93	0.024	1.00	0.24
ILE15	HA	1.00	0.001	1.00	4.24
ILE15	HB	1.00	0.001	1.00	0.35
ILE15	HG12	1.00	0.008	1.00	0.45
ILE15	HG13	1.00	0.002	1.00	0.80
ILE15	HG21	1.00	0.003	1.00	1.13
ILE15	HD11	0.97	0.020	1.00	0.80
ILE15	H	1.00	0.004	1.00	0.44
LYS16	HA	1.00	0.467	0.00	0.00
LYS16	H	1.00	0.003	1.00	0.24

3.15.2 Detailed Probabilities of ILE15CB:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE15	0.71	1.00
LYS16	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I15HA	1.00
I15HG12	1.00
I15HG13	1.00
I15HG21	1.00
I15HD11	1.00
I15H	1.00
I15HB	1.00
K16H	1.00

NOESY contacts detailed probability

3.15 ILE(15)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE15	HA	1.00	0.000	1.00	0.20
ILE15	HB	1.00	0.003	1.00	3.48
ILE15	HG12	1.00	0.011	1.00	0.55
ILE15	HG13	1.00	0.203	0.00	0.00
ILE15	HG21	1.00	0.008	1.00	1.61
ILE15	HD11	1.00	0.075	0.00	0.00
ILE15	H	1.00	0.005	1.00	0.56
LYS16	H	1.00	0.001	1.00	0.42
LYS16	HA	0.88	0.023	1.00	0.05

3.15.3 Detailed Probabilities of ILE15CG1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE15	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I15HA	1.00
I15HB	1.00
I15HG12	1.00
I15HG21	1.00
I15HD11	1.00
I15H	1.00
I15HG13	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE15	HA	1.00	0.005	1.00	0.23
ILE15	HB	1.00	0.001	1.00	0.17
ILE15	HG12	1.00	0.004	1.00	0.63
ILE15	HG13	1.00	0.014	1.00	0.74
ILE15	HG21	1.00	0.008	1.00	0.73
ILE15	HD11	1.00	0.005	1.00	0.95
ILE15	H	1.00	0.004	1.00	0.20

3.15.4 Detailed Probabilities of ILE15CG2:

Overall probability: 0.556

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE15	0.43	1.00
LYS16	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I15HA	1.00
I15HB	1.00
I15HG12	1.00
I15HG13	1.00
I15HG22	1.00
I15HD11	0.99
I15H	1.00
K16H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE15	HA	1.00	0.004	1.00	0.79
ILE15	HB	1.00	0.002	1.00	1.38
ILE15	HG12	1.00	0.097	0.00	0.00
ILE15	HG13	1.00	0.586	0.00	0.00
ILE15	HG21	1.00	0.782	0.00	0.00
ILE15	HD11	0.99	0.714	0.01	0.00
ILE15	H	1.00	0.007	1.00	0.31
LYS16	H	0.98	0.002	1.00	0.36
LYS16	HA	0.65	0.002	1.00	0.25

3.15.5 Detailed Probabilities of ILE15CD1:

Overall probability: 0.575

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE15	0.58	1.00

Expected NOESY Contacts

Proton	Expected probability
I15HA	0.97
I15HB	1.00
I15HG12	1.00
I15HG13	1.00
I15HG21	0.99
I15HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE15	HA	0.97	0.354	0.03	0.00
ILE15	HB	1.00	0.194	0.00	0.00
ILE15	HG12	1.00	0.005	1.00	1.23
ILE15	HG13	1.00	0.026	1.00	2.13
ILE15	HG21	0.99	0.006	1.00	3.89
ILE15	HD11	1.00	0.089	0.00	0.00
ILE15	H	0.94	0.006	1.00	0.50

3.15.6 Detailed Probabilities of ILE15N:

Overall probability: 0.868

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU14	0.72	1.00
ILE15	1.00	1.00
LYS16	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L14HB2	1.00
L14H	1.00
L14HB3	1.00
L14HA	1.00
L14HG	0.99
I15HA	1.00
I15HB	1.00
I15HG12	1.00
I15HG13	1.00
I15HG21	1.00
I15H	1.00
K16H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU14	HA	1.00	0.069	0.00	0.00
LEU14	HB2	1.00	0.005	1.00	-466690.00
LEU14	HB3	1.00	0.026	1.00	-1002986.00
LEU14	HG	0.99	0.094	0.01	0.00
LEU14	H	1.00	0.011	1.00	-1320468.00
LEU14	HD11	0.53	0.007	1.00	-1213214.00
LEU14	HD21	0.63	0.003	1.00	-954284.00
ILE15	HA	1.00	0.002	1.00	-547495.00
ILE15	HB	1.00	0.005	1.00	-1103483.00
ILE15	HG12	1.00	0.008	1.00	-828808.00
ILE15	HG13	1.00	0.007	1.00	-550197.00
ILE15	HG21	1.00	0.019	1.00	-1213214.00
ILE15	H	1.00	0.020	1.00	-14779317.00
ILE15	HD11	0.94	0.004	1.00	-954284.00
LYS16	H	1.00	0.016	1.00	-1320468.00

3.15.7 Detailed Probabilities of ILE15HA:

Overall probability: 0.703

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU14	0.00	1.00
ILE15	0.86	1.00
LYS16	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
L14HA	1.00
I15HB	1.00
I15HG12	1.00
I15HG13	1.00
I15HG21	1.00
I15HD11	0.97
I15H	1.00
I15HA	1.00
K16H	1.00
K16HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU14	HA	1.00	0.356	0.00	0.00
ILE15	HA	1.00	0.001	1.00	4.24
ILE15	HB	1.00	0.000	1.00	0.20
ILE15	HG12	1.00	0.001	1.00	0.22
ILE15	HG13	1.00	0.005	1.00	0.23
ILE15	HG21	1.00	0.004	1.00	0.79
ILE15	HD11	0.97	0.354	0.03	0.00
ILE15	H	1.00	0.002	1.00	-547495.00
LYS16	HA	1.00	0.480	0.00	0.00
LYS16	H	1.00	0.003	1.00	-143935.00

3.15.8 Detailed Probabilities of ILE15HB:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE15	0.71	1.00
LYS16	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I15HA	1.00
I15HG12	1.00
I15HG13	1.00
I15HG21	1.00
I15HD11	1.00
I15H	1.00
I15HB	1.00
K16H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE15	HA	1.00	0.001	1.00	0.35
ILE15	HB	1.00	0.003	1.00	3.48
ILE15	HG12	1.00	1.055	0.00	0.00
ILE15	HG13	1.00	0.001	1.00	0.17
ILE15	HG21	1.00	0.002	1.00	1.38
ILE15	HD11	1.00	0.194	0.00	0.00
ILE15	H	1.00	0.005	1.00	-1103483.00
LYS16	H	1.00	0.013	1.00	-2784560.00
LYS16	HA	0.88	0.003	1.00	3.14

3.15.9 Detailed Probabilities of ILE15HG12:

Overall probability: 0.628

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE15	0.71	1.00
LYS16	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
I15HA	1.00
I15HB	1.00
I15HG13	1.00
I15HG21	1.00
I15HD11	1.00
I15H	1.00
I15HG12	1.00
K16H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE15	HA	1.00	0.008	1.00	0.45
ILE15	HB	1.00	0.011	1.00	0.55
ILE15	HG12	1.00	0.866	0.00	0.00
ILE15	HG13	1.00	0.004	1.00	0.63
ILE15	HG21	1.00	0.097	0.00	0.00
ILE15	HD11	1.00	0.005	1.00	1.23
ILE15	H	1.00	0.008	1.00	-828808.00
LYS16	H	0.98	0.068	0.02	0.00

3.15.10 Detailed Probabilities of ILE15HG13:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE15	0.71	1.00

Expected NOESY Contacts

Proton	Expected probability
I15HA	1.00
I15HB	1.00
I15HG12	1.00
I15HG21	1.00
I15HD11	1.00
I15H	1.00
I15HG13	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE15	HA	1.00	0.002	1.00	0.80
ILE15	HB	1.00	0.203	0.00	0.00
ILE15	HG12	1.00	0.008	1.00	0.69
ILE15	HG13	1.00	0.014	1.00	0.74
ILE15	HG21	1.00	0.586	0.00	0.00
ILE15	HD11	1.00	0.026	1.00	2.13
ILE15	H	1.00	0.007	1.00	-550197.00

3.15.11 Detailed Probabilities of ILE15HG21:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE15	0.86	1.00
LYS16	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I15HA	1.00
I15HB	1.00
I15HG12	1.00
I15HG13	1.00
I15HG22	1.00
I15HD11	0.99
I15H	1.00
K16H	0.98

NOESY contacts detailed probability

3.15 ILE(15)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE15	HA	1.00	0.003	1.00	1.13
ILE15	HB	1.00	0.008	1.00	1.61
ILE15	HG12	1.00	0.013	1.00	0.74
ILE15	HG13	1.00	0.008	1.00	0.73
ILE15	HG21	1.00	0.782	0.00	0.00
ILE15	HD11	0.99	0.006	1.00	3.89
ILE15	H	1.00	0.019	1.00	-1213214.00
LYS16	H	0.98	0.017	1.00	-1748549.00

3.15.12 Detailed Probabilities of ILE15HD11:

Overall probability: 0.572

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE15	0.57	1.00

Expected NOESY Contacts

Proton	Expected probability
I15HA	0.97
I15HB	1.00
I15HG12	1.00
I15HG13	1.00
I15HG21	0.99
I15HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE15	HA	0.97	0.020	1.00	0.80
ILE15	HB	1.00	0.075	0.00	0.00
ILE15	HG12	1.00	0.002	1.00	0.74
ILE15	HG13	1.00	0.005	1.00	0.95
ILE15	HG21	0.99	0.714	0.01	0.00
ILE15	HD11	1.00	0.089	0.00	0.00
ILE15	H	0.94	0.004	1.00	-954284.00

3.15.13 Detailed Probabilities of ILE15H:

Overall probability: 0.786

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU14	0.40	1.00
ILE15	1.00	1.00
LYS16	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L14HB2	1.00
L14H	1.00
L14HB3	1.00
L14HA	1.00
L14HG	0.99
I15HA	1.00
I15HB	1.00
I15HG12	1.00
I15HG13	1.00
I15HG21	1.00
I15H	1.00
K16H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU14	HA	1.00	0.050	0.00	0.00
LEU14	HB2	1.00	0.017	1.00	0.13
LEU14	HB3	1.00	0.661	0.00	0.00
LEU14	HG	0.99	0.010	1.00	0.07
LEU14	H	1.00	0.041	0.00	0.00
ILE15	HA	1.00	0.004	1.00	0.44
ILE15	HB	1.00	0.005	1.00	0.56
ILE15	HG12	1.00	0.004	1.00	0.36
ILE15	HG13	1.00	0.004	1.00	0.20
ILE15	HG21	1.00	0.007	1.00	0.31
ILE15	H	1.00	0.020	1.00	-14779317.00
ILE15	HD11	0.94	0.006	1.00	0.50
LYS16	H	1.00	0.001	1.00	-585214.00
LYS16	HA	0.90	0.027	1.00	0.07

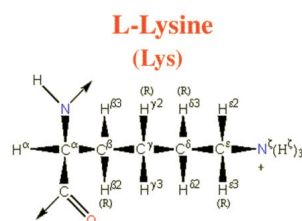


Figure 16: Image from the BMRB

Residue probability: 0.729
 Residue probability confidence: 0.943

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	179.577	176.660	3.133	0.000	0.000
CA 3.16.1	60.169	57.014	3.028	0.654	1.000
CB 3.16.2	32.164	32.981	3.186	0.780	1.000
CG 3.16.3	25.305	24.941	1.956	0.800	0.909
CD 3.16.4	29.236	29.020	2.193	0.667	0.889
CE 3.16.5	41.780	41.893	1.492	0.800	0.875
N 3.16.6	117.596	120.954	4.210	0.880	1.000
NZ	NA	—	—	0.000	0.000
HA 3.16.7	3.843	4.262	0.489	0.857	1.000
HB2 3.16.8	1.880	1.774	0.365	0.470	1.000
HB3 3.16.9	1.881	1.742	0.385	0.490	1.000
HG2 3.16.10	1.627	1.358	0.344	0.433	0.909
HG3 3.16.11	1.396	1.343	0.357	0.610	0.909
HD2 3.16.12	1.685	1.614	0.957	0.750	0.889
HD3 3.16.13	1.688	1.595	0.387	0.750	0.889
HE 3.16.14	2.910	2.907	0.230	1.000	0.875
H 3.16.15	7.604	8.185	0.605	1.000	1.000
HZ	NA	—	—	0.000	0.000

3.16.1 Detailed Probabilities of LYS16CA:

Overall probability: 0.654
 Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE15	0.67	1.00
LYS16	0.69	1.00
LYS17	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
I15HA	1.00
K16HB2	1.00
K16HB3	1.00
K16HG2	1.00
K16HG3	1.00
K16HD2	0.98
K16HD3	0.98
K16H	1.00
K16HA	1.00
K17HA	1.00
K17H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE15	HA	1.00	0.480	0.00	0.00
ILE15	HB	0.88	0.003	1.00	3.14
ILE15	H	0.90	0.027	1.00	0.07
LYS16	HA	1.00	0.007	1.00	20.35
LYS16	HB2	1.00	0.038	0.20	0.00
LYS16	HB3	1.00	0.037	0.30	0.00
LYS16	HG2	1.00	0.010	1.00	0.96
LYS16	HG3	1.00	0.043	0.00	0.00
LYS16	HD2	0.98	0.016	1.00	1.06
LYS16	HD3	0.98	0.013	1.00	1.06
LYS16	H	1.00	0.004	1.00	0.97
LYS17	HA	1.00	0.119	0.00	0.00
LYS17	H	1.00	0.025	1.00	0.97

3.16.2 Detailed Probabilities of LYS16CB:

Overall probability: 0.780

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS16	0.78	1.00
LYS17	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
K16HA	1.00
K16HB3	1.00
K16HG2	1.00
K16HG3	1.00
K16HD2	1.00
K16HD3	1.00
K16HE2	0.98
K16H	1.00
K16HB2	1.00
K17H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS16	HA	1.00	0.022	1.00	2.44
LYS16	HB2	1.00	0.024	1.00	53.87
LYS16	HB3	1.00	0.023	1.00	53.87
LYS16	HG2	1.00	0.154	0.00	0.00
LYS16	HG3	1.00	0.077	0.00	0.00
LYS16	HD2	1.00	0.002	1.00	5.56
LYS16	HD3	1.00	0.005	1.00	5.56
LYS16	HE2	0.98	0.019	1.00	0.70
LYS16	H	1.00	0.011	1.00	2.14
LYS17	H	1.00	0.032	0.80	0.00

3.16.3 Detailed Probabilities of LYS16CG:

Overall probability: 0.800

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS16	0.78	0.90
LYS17	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K16HA	1.00
K16HB2	1.00
K16HB3	1.00
K16HG2	1.00
K16HD2	1.00
K16HD3	1.00
K16HE2	1.00
K16H	1.00
K16HZ2	1.00
K16HG3	1.00
K17H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS16	HA	1.00	0.003	1.00	0.66
LYS16	HB2	1.00	0.021	1.00	0.97
LYS16	HB3	1.00	0.022	1.00	0.97
LYS16	HG2	1.00	0.008	1.00	9.44
LYS16	HG3	1.00	0.012	1.00	36.93
LYS16	HD2	1.00	0.050	0.00	0.00
LYS16	HD3	1.00	0.053	0.00	0.00
LYS16	HE2	1.00	0.013	1.00	0.66
LYS16	H	1.00	0.006	1.00	0.42
LYS17	H	0.96	0.015	1.00	0.42

3.16.4 Detailed Probabilities of LYS16CD:

Overall probability: 0.667

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS16	0.67	0.89

Expected NOESY Contacts

Proton	Expected probability
K16HA	0.98
K16HB2	1.00
K16HB3	1.00
K16HG2	1.00
K16HG3	1.00
K16HD2	1.00
K16HE2	1.00
K16HZ2	1.00
K16HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS16	HA	0.98	0.004	1.00	0.37
LYS16	HB2	1.00	0.052	0.00	0.00
LYS16	HB3	1.00	0.051	0.00	0.00
LYS16	HG2	1.00	0.057	0.00	0.00
LYS16	HG3	1.00	0.007	1.00	6.19
LYS16	HD2	1.00	0.001	1.00	244.35
LYS16	HD3	1.00	0.004	1.00	244.35
LYS16	HE2	1.00	0.003	1.00	4.26
LYS16	H	0.87	0.011	1.00	0.43

3.16.5 Detailed Probabilities of LYS16CE:

Overall probability: 0.800

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS16	0.80	0.88

Expected NOESY Contacts

Proton	Expected probability
K16HB2	0.98
K16HB3	0.99
K16HG2	1.00
K16HG3	1.00
K16HD2	1.00
K16HD3	1.00
K16HE3	1.00
K16HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS16	HB2	0.99	0.035	0.50	0.00
LYS16	HB3	0.99	0.034	0.60	0.00
LYS16	HG2	1.00	0.037	0.30	0.00
LYS16	HG3	1.00	0.015	1.00	1.85
LYS16	HD2	1.00	0.021	1.00	7.15
LYS16	HD3	1.00	0.024	1.00	7.15
LYS16	HE2	1.00	0.007	1.00	220.78
LYS16	HA	0.76	0.012	1.00	0.16

3.16.6 Detailed Probabilities of LYS16N:

Overall probability: 0.880

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE15	0.84	1.00
LYS16	0.88	1.00
LYS17	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I15HG21	0.98
I15HB	1.00
I15HG12	0.98
I15H	1.00
I15HA	1.00
K16HA	1.00
K16HB2	1.00
K16HB3	1.00
K16HG2	1.00
K16HG3	1.00
K16H	1.00
K17H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE15	HA	1.00	0.003	1.00	-143935.00
ILE15	HB	1.00	0.013	1.00	-2784560.00
ILE15	HG12	0.98	0.068	0.02	0.00
ILE15	HG21	0.98	0.017	1.00	-1748549.00
ILE15	H	1.00	0.001	1.00	-585214.00
ILE15	HG13	0.95	0.017	1.00	-146186.00
LYS16	HA	1.00	0.006	1.00	-950003.00
LYS16	HB2	1.00	0.022	1.00	-2784560.00
LYS16	HB3	1.00	0.021	1.00	-2784560.00
LYS16	HG2	1.00	0.014	1.00	-1734049.00
LYS16	HG3	1.00	0.037	0.30	0.00
LYS16	H	1.00	0.006	1.00	-17911656.00
LYS17	H	1.00	0.027	1.00	-17911656.00
LYS17	HA	0.88	0.028	1.00	-495322.00

3.16.7 Detailed Probabilities of LYS16HA:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE15	0.67	1.00
LYS16	1.00	1.00
LYS17	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
I15HA	1.00
K16HB2	1.00
K16HB3	1.00
K16HG2	1.00
K16HG3	1.00
K16HD2	0.98
K16HD3	0.98
K16H	1.00
K16HA	1.00
K17HA	1.00
K17H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE15	HA	1.00	0.467	0.00	0.00
ILE15	HB	0.88	0.023	1.00	0.05
ILE15	HG21	0.68	0.002	1.00	0.25
LYS16	HA	1.00	0.007	1.00	20.35
LYS16	HB2	1.00	0.022	1.00	2.44
LYS16	HB3	1.00	0.022	1.00	2.44
LYS16	HG2	1.00	0.003	1.00	0.35
LYS16	HG3	1.00	0.003	1.00	0.66
LYS16	HD2	0.98	0.004	1.00	0.37
LYS16	HD3	0.98	0.004	1.00	0.37
LYS16	H	1.00	0.006	1.00	-950003.00
LYS16	HE2	0.77	0.012	1.00	0.16
LYS17	HA	1.00	0.096	0.00	0.00
LYS17	H	1.00	0.007	1.00	-236327.00

3.16.8 Detailed Probabilities of LYS16HB2:

Overall probability: 0.470

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS16	0.52	1.00
LYS17	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K16HA	1.00
K16HB3	1.00
K16HG2	1.00
K16HG3	1.00
K16HD2	1.00
K16HD3	1.00
K16HE2	0.98
K16H	1.00
K16HB2	1.00
K17H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS16	HA	1.00	0.038	0.20	0.00
LYS16	HB2	1.00	0.024	1.00	53.87
LYS16	HB3	1.00	0.024	1.00	53.87
LYS16	HG2	1.00	0.255	0.00	0.00
LYS16	HG3	1.00	0.021	1.00	0.97
LYS16	HD2	1.00	0.052	0.00	0.00
LYS16	HD3	1.00	0.052	0.00	0.00
LYS16	HE2	0.98	0.035	0.50	0.00
LYS16	H	1.00	0.022	1.00	-2784560.00
LYS17	H	1.00	0.125	0.00	0.00

3.16.9 Detailed Probabilities of LYS16HB3:

Overall probability: 0.490

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS16	0.54	1.00
LYS17	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K16HA	1.00
K16HB2	1.00
K16HG2	1.00
K16HG3	1.00
K16HD2	1.00
K16HD3	1.00
K16HE2	0.99
K16H	1.00
K16HB3	1.00
K17H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS16	HA	1.00	0.037	0.30	0.00
LYS16	HB2	1.00	0.023	1.00	53.87
LYS16	HB3	1.00	0.023	1.00	53.87
LYS16	HG2	1.00	0.255	0.00	0.00
LYS16	HG3	1.00	0.022	1.00	0.97
LYS16	HD2	1.00	0.051	0.00	0.00
LYS16	HD3	1.00	0.051	0.00	0.00
LYS16	HE2	0.99	0.034	0.60	0.00
LYS16	H	1.00	0.021	1.00	-2784560.00
LYS17	H	1.00	0.126	0.00	0.00

3.16.10 Detailed Probabilities of LYS16HG2:

Overall probability: 0.433

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS16	0.48	0.90
LYS17	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
K16HA	1.00
K16HB2	1.00
K16HB3	1.00
K16HG3	1.00
K16HD2	1.00
K16HD3	1.00
K16HE2	1.00
K16H	1.00
K16HZ2	1.00
K16HG2	1.00
K17H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS16	HA	1.00	0.010	1.00	0.96
LYS16	HB2	1.00	0.154	0.00	0.00
LYS16	HB3	1.00	0.154	0.00	0.00
LYS16	HG2	1.00	0.002	1.00	25.64
LYS16	HG3	1.00	0.008	1.00	9.44
LYS16	HD2	1.00	0.057	0.00	0.00
LYS16	HD3	1.00	0.057	0.00	0.00
LYS16	HE2	1.00	0.037	0.30	0.00
LYS16	H	1.00	0.014	1.00	-1734049.00
LYS17	H	0.97	0.128	0.03	0.00

3.16.11 Detailed Probabilities of LYS16HG3:

Overall probability: 0.610

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS16	0.59	0.90
LYS17	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
K16HA	1.00
K16HB2	1.00
K16HB3	1.00
K16HG2	1.00
K16HD2	1.00
K16HD3	1.00
K16HE2	1.00
K16H	1.00
K16HZ2	1.00
K16HG3	1.00
K17H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS16	HA	1.00	0.043	0.00	0.00
LYS16	HB2	1.00	0.077	0.00	0.00
LYS16	HB3	1.00	0.077	0.00	0.00
LYS16	HG2	1.00	0.008	1.00	7.08
LYS16	HG3	1.00	0.012	1.00	36.93
LYS16	HD2	1.00	0.007	1.00	6.19
LYS16	HD3	1.00	0.007	1.00	6.19
LYS16	HE2	1.00	0.015	1.00	1.85
LYS16	H	1.00	0.037	0.30	0.00
LYS17	H	0.96	0.032	0.80	0.00

3.16.12 Detailed Probabilities of LYS16HD2:

Overall probability: 0.750

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS16	0.75	0.89

Expected NOESY Contacts

Proton	Expected probability
K16HA	0.98
K16HB2	1.00
K16HB3	1.00
K16HG2	1.00
K16HG3	1.00
K16HD3	1.00
K16HE2	1.00
K16HZ2	1.00
K16HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS16	HA	0.98	0.016	1.00	1.06
LYS16	HB2	1.00	0.002	1.00	5.56
LYS16	HB3	1.00	0.002	1.00	5.56
LYS16	HG2	1.00	0.060	0.00	0.00
LYS16	HG3	1.00	0.050	0.00	0.00
LYS16	HD2	1.00	0.001	1.00	244.35
LYS16	HD3	1.00	0.001	1.00	244.35
LYS16	HE2	1.00	0.021	1.00	7.15

3.16.13 Detailed Probabilities of LYS16HD3:

Overall probability: 0.750

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS16	0.75	0.89

Expected NOESY Contacts

Proton	Expected probability
K16HA	0.98
K16HB2	1.00
K16HB3	1.00
K16HG2	1.00
K16HG3	1.00
K16HD2	1.00
K16HE2	1.00
K16HZ2	1.00
K16HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS16	HA	0.98	0.013	1.00	1.06
LYS16	HB2	1.00	0.005	1.00	5.56
LYS16	HB3	1.00	0.005	1.00	5.56
LYS16	HG2	1.00	0.063	0.00	0.00
LYS16	HG3	1.00	0.053	0.00	0.00
LYS16	HD2	1.00	0.004	1.00	244.35
LYS16	HD3	1.00	0.004	1.00	244.35
LYS16	HE2	1.00	0.024	1.00	7.15

3.16.14 Detailed Probabilities of LYS16HE2:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS16	1.00	0.88

Expected NOESY Contacts

Proton	Expected probability
K16HB2	0.98
K16HB3	0.99
K16HG2	1.00
K16HG3	1.00
K16HD2	1.00
K16HD3	1.00
K16HE3	1.00
K16HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS16	HB2	0.99	0.019	1.00	0.70
LYS16	HB3	0.99	0.019	1.00	0.70
LYS16	HG2	1.00	0.012	1.00	0.53
LYS16	HG3	1.00	0.013	1.00	0.66
LYS16	HD2	1.00	0.003	1.00	4.26
LYS16	HD3	1.00	0.003	1.00	4.26
LYS16	HE2	1.00	0.007	1.00	220.78

3.16.15 Detailed Probabilities of LYS16H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE15	1.00	1.00
LYS16	1.00	1.00
LYS17	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I15HG21	0.98
I15HB	1.00
I15HG12	0.98
I15H	1.00
I15HA	1.00
K16HA	1.00
K16HB2	1.00
K16HB3	1.00
K16HG2	1.00
K16HG3	1.00
K16H	1.00
K17H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE15	HA	1.00	0.003	1.00	0.24
ILE15	HB	1.00	0.001	1.00	0.42
ILE15	HG12	0.98	0.013	1.00	0.12
ILE15	HG21	0.98	0.002	1.00	0.36
ILE15	H	1.00	0.016	1.00	-1320468.00
LYS16	HA	1.00	0.004	1.00	0.97
LYS16	HB2	1.00	0.011	1.00	2.14
LYS16	HB3	1.00	0.011	1.00	2.14
LYS16	HG2	1.00	0.003	1.00	0.56
LYS16	HG3	1.00	0.006	1.00	0.42
LYS16	H	1.00	0.006	1.00	-17911656.00
LYS16	HD2	0.88	0.011	1.00	0.43
LYS16	HD3	0.87	0.011	1.00	0.43
LYS17	H	1.00	0.012	1.00	-8033900.00
LYS17	HA	0.88	0.009	1.00	0.63
LYS17	HB2	0.61	0.014	1.00	0.34

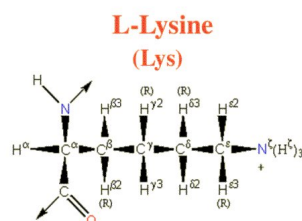


Figure 17: Image from the BMRB

Residue probability: 0.527
Residue probability confidence: 0.945

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	179.380	176.660	3.133	0.000	0.000
CA 3.17.1	59.840	57.014	3.028	0.583	1.000
CB 3.17.2	33.065	32.981	3.186	0.093	1.000
CG 3.17.3	25.822	24.941	1.956	0.639	0.917
CD 3.17.4	29.705	29.020	2.193	0.600	0.900
CE 3.17.5	41.780	41.893	1.492	0.878	0.889
N 3.17.6	118.832	120.954	4.210	0.602	1.000
NZ	NA	—	—	0.000	0.000
HA 3.17.7	3.992	4.262	0.489	0.644	1.000
HB2 3.17.8	1.993	1.774	0.365	0.168	1.000
HB3 3.17.9	1.922	1.742	0.385	0.636	1.000
HG2 3.17.10	1.755	1.358	0.344	0.094	0.917
HG3 3.17.11	1.429	1.343	0.357	0.700	0.917
HD2 3.17.12	1.680	1.614	0.957	0.433	0.900
HD3 3.17.13	1.517	1.595	0.387	0.444	0.900
HE2 3.17.14	2.848	2.907	0.230	0.378	0.889
HE3 3.17.15	2.900	2.901	0.241	0.628	0.889
H 3.17.16	7.583	8.185	0.605	0.911	1.000
HZ	NA	—	—	0.000	0.000

3.17.1 Detailed Probabilities of LYS17CA:

Overall probability: 0.583
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS16	0.50	1.00
LYS17	0.63	1.00
ILE18	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K16HA	1.00
K17HB2	1.00
K17HB3	1.00
K17HG2	1.00
K17HG3	1.00
K17HD2	0.98
K17HD3	0.98
K17H	1.00
K17HA	1.00
I18HA	1.00
I18H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS16	HA	1.00	0.096	0.00	0.00
LYS16	H	0.88	0.009	1.00	0.63
LYS17	HA	1.00	0.245	0.00	0.00
LYS17	HB2	1.00	0.052	0.00	0.00
LYS17	HB3	1.00	0.019	1.00	3.48
LYS17	HG2	1.00	0.054	0.00	0.00
LYS17	HG3	1.00	0.025	1.00	1.34
LYS17	HD2	0.98	0.021	1.00	1.39
LYS17	HD3	0.98	0.006	1.00	0.56
LYS17	H	1.00	0.012	1.00	0.63
ILE18	HA	1.00	0.375	0.00	0.00
ILE18	H	1.00	0.005	1.00	0.23

3.17.2 Detailed Probabilities of LYS17CB:

Overall probability: 0.093

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS17	0.10	1.00
ILE18	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K17HA	1.00
K17HB3	1.00
K17HG2	1.00
K17HG3	1.00
K17HD2	1.00
K17HD3	1.00
K17HE2	0.98
K17HE3	0.99
K17H	1.00
K17HB2	1.00
I18H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS17	HA	1.00	0.678	0.00	0.00
LYS17	HB2	1.00	1.326	0.00	0.00
LYS17	HB3	1.00	1.255	0.00	0.00
LYS17	HG2	1.00	1.088	0.00	0.00
LYS17	HG3	1.00	0.762	0.00	0.00
LYS17	HD2	1.00	1.013	0.00	0.00
LYS17	HD3	1.00	0.850	0.00	0.00
LYS17	HE2	0.98	1.822	0.02	0.00
LYS17	HE3	0.99	1.770	0.01	0.00
LYS17	H	1.00	0.007	1.00	0.34
ILE18	H	1.00	1.195	0.00	0.00

3.17.3 Detailed Probabilities of LYS17CG:

Overall probability: 0.639

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS17	0.70	0.91
ILE18	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
K17HA	1.00
K17HB2	1.00
K17HB3	1.00
K17HG3	1.00
K17HD2	1.00
K17HD3	1.00
K17HE2	1.00
K17HE3	1.00
K17H	1.00
K17HZ2	1.00
K17HG2	1.00
I18H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS17	HA	1.00	0.003	1.00	0.39
LYS17	HB2	1.00	0.095	0.00	0.00
LYS17	HB3	1.00	0.024	1.00	0.68
LYS17	HG2	1.00	0.143	0.00	0.00
LYS17	HG3	1.00	0.014	1.00	1.43
LYS17	HD2	1.00	0.161	0.00	0.00
LYS17	HD3	1.00	0.002	1.00	0.55
LYS17	HE2	1.00	0.002	1.00	0.24
LYS17	HE3	1.00	0.004	1.00	0.23
LYS17	H	1.00	0.007	1.00	0.35
ILE18	H	0.97	1.195	0.03	0.00

3.17.4 Detailed Probabilities of LYS17CD:

Overall probability: 0.600

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS17	0.60	0.90

Expected NOESY Contacts

Proton	Expected probability
K17HA	0.98
K17HB2	1.00
K17HB3	1.00
K17HG2	1.00
K17HG3	1.00
K17HD2	1.00
K17HE2	1.00
K17HE3	1.00
K17HZ2	1.00
K17HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS17	HA	0.98	0.005	1.00	0.37
LYS17	HB2	1.00	0.045	0.00	0.00
LYS17	HB3	1.00	0.026	1.00	0.43
LYS17	HG2	1.00	0.193	0.00	0.00
LYS17	HG3	1.00	0.014	1.00	0.93
LYS17	HD2	1.00	0.265	0.00	0.00
LYS17	HD3	1.00	0.102	0.00	0.00
LYS17	HE2	1.00	0.006	1.00	0.22
LYS17	HE3	1.00	0.017	1.00	0.45
LYS17	H	0.87	0.008	1.00	0.15

3.17.5 Detailed Probabilities of LYS17CE:

Overall probability: 0.878

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS17	0.88	0.89

Expected NOESY Contacts

Proton	Expected probability
K17HB2	0.98
K17HB3	0.99
K17HG2	1.00
K17HG3	1.00
K17HD2	1.00
K17HD3	1.00
K17HE3	1.00
K17HZ2	1.00
K17HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS17	HB2	0.98	0.008	1.00	0.22
LYS17	HB3	0.99	0.003	1.00	0.28
LYS17	HG2	1.00	0.106	0.00	0.00
LYS17	HG3	1.00	0.008	1.00	0.59
LYS17	HD2	1.00	0.031	0.90	0.00
LYS17	HD3	1.00	0.029	1.00	1.11
LYS17	HE2	1.00	0.022	1.00	46.58
LYS17	HE3	1.00	0.030	1.00	46.58
LYS17	HA	0.77	0.010	1.00	0.21

3.17.6 Detailed Probabilities of LYS17N:

Overall probability: 0.602

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS16	0.47	1.00
LYS17	0.67	1.00
ILE18	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K16HB2	1.00
K16HG3	0.96
K16HB3	1.00
K16HA	1.00
K16HG2	0.97
K16H	1.00
K17HA	1.00
K17HB2	1.00
K17HB3	1.00
K17HG2	1.00
K17HG3	1.00
K17H	1.00
I18H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS16	HA	1.00	0.007	1.00	-236327.00
LYS16	HB2	1.00	0.125	0.00	0.00
LYS16	HB3	1.00	0.126	0.00	0.00
LYS16	HG2	0.97	0.128	0.03	0.00
LYS16	HG3	0.96	0.032	0.80	0.00
LYS16	H	1.00	0.012	1.00	-8033900.00
LYS17	HA	1.00	0.004	1.00	-940566.00
LYS17	HB2	1.00	0.238	0.00	0.00
LYS17	HB3	1.00	0.167	0.00	0.00
LYS17	HG2	1.00	0.000	1.00	-858198.00
LYS17	HG3	1.00	0.001	1.00	-514633.00
LYS17	H	1.00	0.009	1.00	-8033900.00
ILE18	H	1.00	0.004	1.00	-729370.00

3.17.7 Detailed Probabilities of LYS17HA:

Overall probability: 0.644

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS16	0.50	1.00
LYS17	0.60	1.00
ILE18	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K16HA	1.00
K17HB2	1.00
K17HB3	1.00
K17HG2	1.00
K17HG3	1.00
K17HD2	0.98
K17HD3	0.98
K17H	1.00
K17HA	1.00
I18HA	1.00
I18H	1.00

NOESY contacts detailed probability

3.17 LYS(17)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS16	HA	1.00	0.119	0.00	0.00
LYS16	H	0.88	0.028	1.00	-495322.00
LYS17	HA	1.00	0.245	0.00	0.00
LYS17	HB2	1.00	0.678	0.00	0.00
LYS17	HB3	1.00	2.786	0.00	0.00
LYS17	HG2	1.00	0.003	1.00	0.39
LYS17	HG3	1.00	0.006	1.00	0.59
LYS17	HD2	0.98	0.056	0.02	0.00
LYS17	HD3	0.98	0.005	1.00	0.37
LYS17	H	1.00	0.004	1.00	-940566.00
LYS17	HE2	0.77	0.010	1.00	0.21
LYS17	HE3	0.76	0.020	1.00	0.74
ILE18	HA	1.00	0.017	1.00	0.11
ILE18	H	1.00	0.000	1.00	-283660.00

3.17.8 Detailed Probabilities of LYS17HB2:

Overall probability: 0.168

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS17	0.10	1.00
ILE18	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K17HA	1.00
K17HB3	1.00
K17HG2	1.00
K17HG3	1.00
K17HD2	1.00
K17HD3	1.00
K17HE2	0.98
K17HE3	0.99
K17H	1.00
K17HB2	1.00
I18H	1.00

NOESY contacts detailed probability

3.17 LYS(17)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS17	HA	1.00	0.052	0.00	0.00
LYS17	HB2	1.00	1.326	0.00	0.00
LYS17	HB3	1.00	0.875	0.00	0.00
LYS17	HG2	1.00	0.095	0.00	0.00
LYS17	HG3	1.00	0.969	0.00	0.00
LYS17	HD2	1.00	0.061	0.00	0.00
LYS17	HD3	1.00	0.045	0.00	0.00
LYS17	HE2	0.98	0.008	1.00	0.22
LYS17	HE3	0.99	0.041	0.01	0.00
LYS17	H	1.00	0.238	0.00	0.00
ILE18	H	1.00	0.053	0.00	0.00
ILE18	HA	0.67	0.019	1.00	0.37

3.17.9 Detailed Probabilities of LYS17HB3:

Overall probability: 0.636

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS17	0.60	1.00
ILE18	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K17HA	1.00
K17HB2	1.00
K17HG2	1.00
K17HG3	1.00
K17HD2	1.00
K17HD3	1.00
K17HE2	0.99
K17HE3	0.99
K17H	1.00
K17HB3	1.00
I18H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS17	HA	1.00	0.019	1.00	3.48
LYS17	HB2	1.00	1.255	0.00	0.00
LYS17	HB3	1.00	0.804	0.00	0.00
LYS17	HG2	1.00	0.024	1.00	0.68
LYS17	HG3	1.00	0.898	0.00	0.00
LYS17	HD2	1.00	0.010	1.00	5.45
LYS17	HD3	1.00	0.026	1.00	0.43
LYS17	HE2	0.99	0.003	1.00	0.28
LYS17	HE3	0.99	0.007	1.00	1.28
LYS17	H	1.00	0.167	0.00	0.00
ILE18	H	1.00	0.018	1.00	-442396.00

3.17.10 Detailed Probabilities of LYS17HG2:

Overall probability: 0.094

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS17	0.10	0.91
ILE18	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
K17HA	1.00
K17HB2	1.00
K17HB3	1.00
K17HG3	1.00
K17HD2	1.00
K17HD3	1.00
K17HE2	1.00
K17HE3	1.00
K17H	1.00
K17HZ2	1.00
K17HG2	1.00
I18H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS17	HA	1.00	0.054	0.00	0.00
LYS17	HB2	1.00	1.088	0.00	0.00
LYS17	HB3	1.00	0.637	0.00	0.00
LYS17	HG2	1.00	0.143	0.00	0.00
LYS17	HG3	1.00	0.731	0.00	0.00
LYS17	HD2	1.00	0.177	0.00	0.00
LYS17	HD3	1.00	0.193	0.00	0.00
LYS17	HE2	1.00	0.106	0.00	0.00
LYS17	HE3	1.00	0.091	0.00	0.00
LYS17	H	1.00	0.000	1.00	-858198.00
ILE18	H	0.97	0.053	0.03	0.00

3.17.11 Detailed Probabilities of LYS17HG3:

Overall probability: 0.700

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS17	0.70	0.91
ILE18	0.70	1.00

Expected NOESY Contacts

Proton	Expected probability
K17HA	1.00
K17HB2	1.00
K17HB3	1.00
K17HG2	1.00
K17HD2	1.00
K17HD3	1.00
K17HE2	1.00
K17HE3	1.00
K17H	1.00
K17HZ2	1.00
K17HG3	1.00
I18H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS17	HA	1.00	0.025	1.00	1.34
LYS17	HB2	1.00	0.762	0.00	0.00
LYS17	HB3	1.00	0.311	0.00	0.00
LYS17	HG2	1.00	0.014	1.00	1.43
LYS17	HG3	1.00	0.405	0.00	0.00
LYS17	HD2	1.00	0.026	1.00	6.19
LYS17	HD3	1.00	0.014	1.00	0.93
LYS17	HE2	1.00	0.008	1.00	0.59
LYS17	HE3	1.00	0.018	1.00	1.85
LYS17	H	1.00	0.001	1.00	-514633.00
ILE18	H	0.96	0.033	0.70	0.00

3.17.12 Detailed Probabilities of LYS17HD2:

Overall probability: 0.433

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS17	0.43	0.90

Expected NOESY Contacts

Proton	Expected probability
K17HA	0.98
K17HB2	1.00
K17HB3	1.00
K17HG2	1.00
K17HG3	1.00
K17HD3	1.00
K17HE2	1.00
K17HE3	1.00
K17HZ2	1.00
K17HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS17	HA	0.98	0.021	1.00	1.39
LYS17	HB2	1.00	1.013	0.00	0.00
LYS17	HB3	1.00	0.562	0.00	0.00
LYS17	HG2	1.00	0.161	0.00	0.00
LYS17	HG3	1.00	0.656	0.00	0.00
LYS17	HD2	1.00	0.004	1.00	244.35
LYS17	HD3	1.00	0.265	0.00	0.00
LYS17	HE2	1.00	0.031	0.90	0.00
LYS17	HE3	1.00	0.016	1.00	7.15

3.17.13 Detailed Probabilities of LYS17HD3:

Overall probability: 0.444

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS17	0.44	0.90

Expected NOESY Contacts

Proton	Expected probability
K17HA	0.98
K17HB2	1.00
K17HB3	1.00
K17HG2	1.00
K17HG3	1.00
K17HD2	1.00
K17HE2	1.00
K17HE3	1.00
K17HZ2	1.00
K17HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS17	HA	0.98	0.006	1.00	0.56
LYS17	HB2	1.00	0.850	0.00	0.00
LYS17	HB3	1.00	0.399	0.00	0.00
LYS17	HG2	1.00	0.002	1.00	0.55
LYS17	HG3	1.00	0.493	0.00	0.00
LYS17	HD2	1.00	0.020	1.00	11.42
LYS17	HD3	1.00	0.102	0.00	0.00
LYS17	HE2	1.00	0.029	1.00	1.11
LYS17	HE3	1.00	0.043	0.00	0.00

3.17.14 Detailed Probabilities of LYS17HE2:

Overall probability: 0.378

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS17	0.38	0.89

Expected NOESY Contacts

Proton	Expected probability
K17HB2	0.98
K17HB3	0.99
K17HG2	1.00
K17HG3	1.00
K17HD2	1.00
K17HD3	1.00
K17HE3	1.00
K17HZ2	1.00
K17HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS17	HB2	0.98	1.822	0.02	0.00
LYS17	HB3	0.99	1.730	0.01	0.00
LYS17	HG2	1.00	0.002	1.00	0.24
LYS17	HG3	1.00	0.992	0.00	0.00
LYS17	HD2	1.00	0.065	0.00	0.00
LYS17	HD3	1.00	0.006	1.00	0.22
LYS17	HE2	1.00	0.022	1.00	46.58
LYS17	HE3	1.00	0.069	0.00	0.00

3.17.15 Detailed Probabilities of LYS17HE3:

Overall probability: 0.628

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS17	0.63	0.89

Expected NOESY Contacts

Proton	Expected probability
K17HB2	0.99
K17HB3	0.99
K17HG2	1.00
K17HG3	1.00
K17HD2	1.00
K17HD3	1.00
K17HE2	1.00
K17HZ2	1.00
K17HE3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS17	HB2	0.99	1.770	0.01	0.00
LYS17	HB3	0.99	1.782	0.01	0.00
LYS17	HG2	1.00	0.004	1.00	0.23
LYS17	HG3	1.00	0.940	0.00	0.00
LYS17	HD2	1.00	0.013	1.00	4.26
LYS17	HD3	1.00	0.017	1.00	0.45
LYS17	HE2	1.00	0.030	1.00	46.58
LYS17	HE3	1.00	0.017	1.00	220.78

3.17.16 Detailed Probabilities of LYS17H:

Overall probability: 0.911

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS16	0.95	1.00
LYS17	0.86	1.00
ILE18	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K16HB2	1.00
K16HG3	0.96
K16HB3	1.00
K16HA	1.00
K16HG2	0.97
K16H	1.00
K17HA	1.00
K17HB2	1.00
K17HB3	1.00
K17HG2	1.00
K17HG3	1.00
K17H	1.00
I18H	1.00

NOESY contacts detailed probability

3.17 LYS(17)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS16	HA	1.00	0.025	1.00	0.97
LYS16	HB2	1.00	0.032	0.80	0.00
LYS16	HB3	1.00	0.032	0.80	0.00
LYS16	HG2	0.97	0.024	1.00	0.56
LYS16	HG3	0.96	0.015	1.00	0.42
LYS16	H	1.00	0.027	1.00	-17911656.00
LYS16	HD2	0.56	0.030	1.00	0.00
LYS16	HD3	0.59	0.030	1.00	0.00
LYS17	HA	1.00	0.012	1.00	0.63
LYS17	HB2	1.00	0.007	1.00	0.34
LYS17	HB3	1.00	0.805	0.00	0.00
LYS17	HG2	1.00	0.007	1.00	0.35
LYS17	HG3	1.00	0.005	1.00	0.30
LYS17	H	1.00	0.009	1.00	-8033900.00
LYS17	HD2	0.88	0.032	0.88	0.00
LYS17	HD3	0.87	0.008	1.00	0.15
ILE18	H	1.00	0.007	1.00	-910247.00

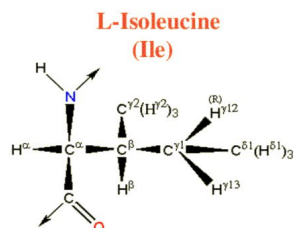


Figure 18: Image from the BMRB

Residue probability: 0.743
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	176.967	175.926	2.710	0.000	0.000
CA 3.18.1	65.474	61.717	4.152	0.811	1.000
CB 3.18.2	37.556	38.702	3.945	0.750	1.000
CG1 3.18.3	29.494	27.785	2.037	0.857	1.000
CG2 3.18.4	17.360	17.574	1.928	0.376	1.000
CD1 3.18.5	13.410	13.545	3.646	0.929	1.000
N 3.18.6	120.961	121.467	6.098	0.782	1.000
HA 3.18.7	3.372	4.185	1.403	0.700	1.000
HB 3.18.8	1.821	1.776	0.310	0.767	1.000
HG12 3.18.9	1.765	1.271	0.411	0.315	1.000
HG13 3.18.10	0.729	1.186	0.426	1.000	1.000
HG2 3.18.11	0.718	0.762	0.283	1.000	1.000
HD1 3.18.12	0.613	0.668	0.293	0.576	1.000
H 3.18.13	8.785	8.301	0.685	0.802	1.000

3.18.1 Detailed Probabilities of ILE18CA:

Overall probability: 0.811
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS17	1.00	1.00
ILE18	0.85	1.00
LYS19	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K17HA	1.00
I18HB	1.00
I18HG12	1.00
I18HG13	1.00
I18HG21	1.00
I18HD11	0.97
I18H	1.00
I18HA	1.00
K19H	1.00
K19HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS17	HA	1.00	0.017	1.00	0.11
LYS17	HB2	0.67	0.019	1.00	0.37
ILE18	HA	1.00	0.006	1.00	4.87
ILE18	HB	1.00	0.031	0.90	0.00
ILE18	HG12	1.00	0.025	1.00	0.55
ILE18	HG13	1.00	0.007	1.00	1.63
ILE18	HG21	1.00	0.004	1.00	1.63
ILE18	HD11	0.97	0.109	0.03	0.00
ILE18	H	1.00	0.002	1.00	0.40
LYS19	HA	1.00	0.295	0.00	0.00
LYS19	H	1.00	0.010	1.00	0.13

3.18.2 Detailed Probabilities of ILE18CB:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE18	0.71	1.00
LYS19	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I18HA	1.00
I18HG12	1.00
I18HG13	1.00
I18HG21	1.00
I18HD11	1.00
I18H	1.00
I18HB	1.00
K19H	1.00

NOESY contacts detailed probability

3.18 ILE(18)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE18	HA	1.00	0.007	1.00	0.24
ILE18	HB	1.00	0.002	1.00	5.18
ILE18	HG12	1.00	0.054	0.00	0.00
ILE18	HG13	1.00	0.011	1.00	1.72
ILE18	HG21	1.00	0.000	1.00	1.72
ILE18	HD11	1.00	0.105	0.00	0.00
ILE18	H	1.00	0.004	1.00	0.67
LYS19	H	1.00	0.011	1.00	0.34

3.18.3 Detailed Probabilities of ILE18CG1:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE18	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
I18HA	1.00
I18HB	1.00
I18HG12	1.00
I18HG21	1.00
I18HD11	1.00
I18H	1.00
I18HG13	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE18	HA	1.00	0.006	1.00	0.21
ILE18	HB	1.00	0.049	0.00	0.00
ILE18	HG12	1.00	0.007	1.00	0.67
ILE18	HG13	1.00	0.010	1.00	1.22
ILE18	HG21	1.00	0.021	1.00	1.22
ILE18	HD11	1.00	0.010	1.00	0.59
ILE18	H	1.00	0.008	1.00	0.16

3.18.4 Detailed Probabilities of ILE18CG2:

Overall probability: 0.376

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE18	0.29	1.00
LYS19	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I18HA	1.00
I18HB	1.00
I18HG12	1.00
I18HG13	1.00
I18HG22	1.00
I18HD11	0.99
I18H	1.00
K19H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE18	HA	1.00	0.405	0.00	0.00
ILE18	HB	1.00	0.054	0.00	0.00
ILE18	HG12	1.00	0.077	0.00	0.00
ILE18	HG13	1.00	0.026	1.00	37.91
ILE18	HG21	1.00	0.015	1.00	37.91
ILE18	HD11	0.99	0.090	0.01	0.00
ILE18	H	1.00	0.148	0.00	0.00
LYS19	H	0.98	0.016	1.00	0.61

3.18.5 Detailed Probabilities of ILE18CD1:

Overall probability: 0.929

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE18	0.93	1.00

Expected NOESY Contacts

Proton	Expected probability
I18HA	0.97
I18HB	1.00
I18HG12	1.00
I18HG13	1.00
I18HG21	0.99
I18HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE18	HA	0.97	0.007	1.00	0.46
ILE18	HB	1.00	0.021	1.00	2.88
ILE18	HG12	1.00	0.035	0.50	0.00
ILE18	HG13	1.00	0.009	1.00	10.40
ILE18	HG21	0.99	0.020	1.00	10.40
ILE18	HD11	1.00	0.010	1.00	90.84
ILE18	H	0.94	0.006	1.00	0.59

3.18.6 Detailed Probabilities of ILE18N:

Overall probability: 0.782

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS17	0.68	1.00
ILE18	0.86	1.00
LYS19	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K17H	1.00
K17HG2	0.97
K17HG3	0.96
K17HA	1.00
K17HB2	1.00
K17HB3	1.00
I18HA	1.00
I18HB	1.00
I18HG12	1.00
I18HG13	1.00
I18HG21	1.00
I18H	1.00
K19H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS17	HA	1.00	0.000	1.00	-283660.00
LYS17	HB2	1.00	0.053	0.00	0.00
LYS17	HB3	1.00	0.018	1.00	-442396.00
LYS17	HG2	0.97	0.053	0.03	0.00
LYS17	HG3	0.96	0.033	0.70	0.00
LYS17	H	1.00	0.007	1.00	-910247.00
LYS17	HD3	0.55	0.026	1.00	-71889.00
ILE18	HA	1.00	0.006	1.00	-549284.00
ILE18	HB	1.00	0.013	1.00	-1353454.00
ILE18	HG12	1.00	0.043	0.00	0.00
ILE18	HG13	1.00	0.002	1.00	-1027950.00
ILE18	HG21	1.00	0.009	1.00	-1027950.00
ILE18	H	1.00	0.003	1.00	-4976595.00
ILE18	HD11	0.94	0.019	1.00	-513549.00
LYS19	H	1.00	0.007	1.00	-580792.00

3.18.7 Detailed Probabilities of ILE18HA:

Overall probability: 0.700

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS17	0.00	1.00
ILE18	0.86	1.00
LYS19	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K17HA	1.00
I18HB	1.00
I18HG12	1.00
I18HG13	1.00
I18HG21	1.00
I18HD11	0.97
I18H	1.00
I18HA	1.00
K19H	1.00
K19HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS17	HA	1.00	0.375	0.00	0.00
ILE18	HA	1.00	0.006	1.00	4.87
ILE18	HB	1.00	0.007	1.00	0.24
ILE18	HG12	1.00	0.006	1.00	0.19
ILE18	HG13	1.00	0.006	1.00	0.21
ILE18	HG21	1.00	0.405	0.00	0.00
ILE18	HD11	0.97	0.007	1.00	0.46
ILE18	H	1.00	0.006	1.00	-549284.00
LYS19	HA	1.00	0.312	0.00	0.00
LYS19	H	1.00	0.005	1.00	-164697.00

3.18.8 Detailed Probabilities of ILE18HB:

Overall probability: 0.767

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE18	0.70	1.00
LYS19	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I18HA	1.00
I18HG12	1.00
I18HG13	1.00
I18HG21	1.00
I18HD11	1.00
I18H	1.00
I18HB	1.00
K19H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE18	HA	1.00	0.031	0.90	0.00
ILE18	HB	1.00	0.002	1.00	5.18
ILE18	HG12	1.00	0.019	1.00	4.53
ILE18	HG13	1.00	0.049	0.00	0.00
ILE18	HG21	1.00	0.054	0.00	0.00
ILE18	HD11	1.00	0.021	1.00	2.88
ILE18	H	1.00	0.013	1.00	-1353454.00
LYS19	H	1.00	0.006	1.00	-1299732.00
LYS19	HA	0.88	0.003	1.00	0.71

3.18.9 Detailed Probabilities of ILE18HG12:

Overall probability: 0.315

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE18	0.36	1.00
LYS19	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
I18HA	1.00
I18HB	1.00
I18HG13	1.00
I18HG21	1.00
I18HD11	1.00
I18H	1.00
I18HG12	1.00
K19H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE18	HA	1.00	0.025	1.00	0.55
ILE18	HB	1.00	0.054	0.00	0.00
ILE18	HG12	1.00	0.075	0.00	0.00
ILE18	HG13	1.00	0.007	1.00	0.67
ILE18	HG21	1.00	0.077	0.00	0.00
ILE18	HD11	1.00	0.035	0.50	0.00
ILE18	H	1.00	0.043	0.00	0.00
LYS19	H	0.98	0.047	0.02	0.00

3.18.10 Detailed Probabilities of ILE18HG13:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE18	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I18HA	1.00
I18HB	1.00
I18HG12	1.00
I18HG21	1.00
I18HD11	1.00
I18H	1.00
I18HG13	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE18	HA	1.00	0.007	1.00	1.63
ILE18	HB	1.00	0.011	1.00	1.72
ILE18	HG12	1.00	0.000	1.00	1.23
ILE18	HG13	1.00	0.010	1.00	1.22
ILE18	HG21	1.00	0.026	1.00	37.91
ILE18	HD11	1.00	0.009	1.00	10.40
ILE18	H	1.00	0.002	1.00	-1027950.00

3.18.11 Detailed Probabilities of ILE18HG21:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE18	1.00	1.00
LYS19	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I18HA	1.00
I18HB	1.00
I18HG12	1.00
I18HG13	1.00
I18HG22	1.00
I18HD11	0.99
I18H	1.00
K19H	0.98

NOESY contacts detailed probability

3.18 ILE(18)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE18	HA	1.00	0.004	1.00	1.63
ILE18	HB	1.00	0.000	1.00	1.72
ILE18	HG12	1.00	0.011	1.00	1.23
ILE18	HG13	1.00	0.021	1.00	1.22
ILE18	HG21	1.00	0.015	1.00	37.91
ILE18	HD11	0.99	0.020	1.00	10.40
ILE18	H	1.00	0.009	1.00	-1027950.00
LYS19	H	0.98	0.007	1.00	-605560.00
LYS19	HA	0.65	0.010	1.00	0.53

3.18.12 Detailed Probabilities of ILE18HD11:

Overall probability: 0.576

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE18	0.58	1.00

Expected NOESY Contacts

Proton	Expected probability
I18HA	0.97
I18HB	1.00
I18HG12	1.00
I18HG13	1.00
I18HG21	0.99
I18HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE18	HA	0.97	0.109	0.03	0.00
ILE18	HB	1.00	0.105	0.00	0.00
ILE18	HG12	1.00	0.016	1.00	0.73
ILE18	HG13	1.00	0.010	1.00	0.59
ILE18	HG21	0.99	0.090	0.01	0.00
ILE18	HD11	1.00	0.010	1.00	90.84
ILE18	H	0.94	0.019	1.00	-513549.00

3.18.13 Detailed Probabilities of ILE18H:

Overall probability: 0.802

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS17	0.72	1.00
ILE18	0.86	1.00
LYS19	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K17H	1.00
K17HG2	0.97
K17HG3	0.96
K17HA	1.00
K17HB2	1.00
K17HB3	1.00
I18HA	1.00
I18HB	1.00
I18HG12	1.00
I18HG13	1.00
I18HG21	1.00
I18H	1.00
K19H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS17	HA	1.00	0.005	1.00	0.23
LYS17	HB2	1.00	1.195	0.00	0.00
LYS17	HB3	1.00	0.014	1.00	1.02
LYS17	HG2	0.97	1.195	0.03	0.00
LYS17	HG3	0.96	0.011	1.00	0.06
LYS17	H	1.00	0.004	1.00	-729370.00
LYS17	HD2	0.54	0.027	1.00	0.16
ILE18	HA	1.00	0.002	1.00	0.40
ILE18	HB	1.00	0.004	1.00	0.67
ILE18	HG12	1.00	0.010	1.00	0.28
ILE18	HG13	1.00	0.008	1.00	0.16
ILE18	HG21	1.00	0.148	0.00	0.00
ILE18	H	1.00	0.003	1.00	-4976595.00
ILE18	HD11	0.94	0.006	1.00	0.59
LYS19	H	1.00	0.005	1.00	-655058.00

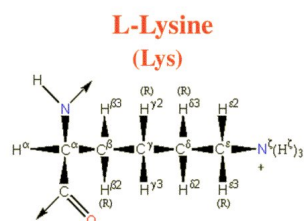
3.19 LYS(19)

Figure 19: Image from the BMRB

Residue probability: 0.807

Residue probability confidence: 0.940

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	177.746	176.660	3.133	0.000	0.000
CA 3.19.1	60.853	57.014	3.028	0.877	1.000
CB 3.19.2	32.326	32.981	3.186	0.778	1.000
CG 3.19.3	27.091	24.941	1.956	0.826	0.900
CD 3.19.4	29.871	29.020	2.193	0.750	0.875
CE 3.19.5	41.780	41.893	1.492	0.967	0.857
N 3.19.6	118.324	120.954	4.210	0.930	1.000
NZ	NA	—	—	0.000	0.000
HA 3.19.7	3.680	4.262	0.489	0.900	1.000
HB2 3.19.8	1.788	1.774	0.365	0.400	1.000
HB3 3.19.9	1.834	1.742	0.385	0.556	1.000
HG2 3.19.10	1.098	1.358	0.344	1.000	0.900
HG3 3.19.11	1.596	1.343	0.357	0.778	0.900
HD 3.19.12	1.594	1.614	0.957	0.750	0.875
HE 3.19.13	2.699	2.907	0.230	0.859	0.857
H 3.19.14	8.532	8.185	0.605	0.930	1.000
HZ	NA	—	—	0.000	0.000

3.19.1 Detailed Probabilities of LYS19CA:

Overall probability: 0.877

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE18	0.67	1.00
LYS19	0.92	1.00
LYS20	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I18HA	1.00
K19HB2	1.00
K19HB3	1.00
K19HG2	1.00
K19HG3	1.00
K19HD2	0.98
K19H	1.00
K19HA	1.00
K20HA	1.00
K20H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE18	HA	1.00	0.312	0.00	0.00
ILE18	HB	0.88	0.003	1.00	0.71
ILE18	HG21	0.68	0.010	1.00	0.53
LYS19	HA	1.00	0.004	1.00	4.48
LYS19	HB2	1.00	0.036	0.40	0.00
LYS19	HB3	1.00	0.010	1.00	0.71
LYS19	HG2	1.00	0.001	1.00	0.42
LYS19	HG3	1.00	0.003	1.00	0.54
LYS19	HD2	0.98	0.005	1.00	0.54
LYS19	H	1.00	0.009	1.00	0.36
LYS19	HE2	0.77	0.001	1.00	0.10
LYS20	HA	1.00	0.016	1.00	0.06
LYS20	H	1.00	0.007	1.00	0.16

3.19.2 Detailed Probabilities of LYS19CB:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS19	0.75	1.00
LYS20	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K19HA	1.00
K19HB3	1.00
K19HG2	1.00
K19HG3	1.00
K19HD2	1.00
K19HE2	0.98
K19H	1.00
K19HB2	1.00
K20H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS19	HA	1.00	0.005	1.00	0.35
LYS19	HB2	1.00	0.092	0.00	0.00
LYS19	HB3	1.00	0.046	0.00	0.00
LYS19	HG2	1.00	0.014	1.00	0.26
LYS19	HG3	1.00	0.000	1.00	1.03
LYS19	HD2	1.00	0.002	1.00	1.03
LYS19	HE2	0.98	0.008	1.00	0.10
LYS19	H	1.00	0.013	1.00	0.26
LYS20	H	1.00	0.001	1.00	0.15

3.19.3 Detailed Probabilities of LYS19CG:

Overall probability: 0.826

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS19	0.92	0.89
LYS20	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
K19HA	1.00
K19HB2	1.00
K19HB3	1.00
K19HG3	1.00
K19HD2	1.00
K19HE2	1.00
K19H	1.00
K19HZ2	1.00
K19HG2	1.00
K20H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS19	HA	1.00	0.001	1.00	0.30
LYS19	HB2	1.00	0.036	0.40	0.00
LYS19	HB3	1.00	0.010	1.00	0.36
LYS19	HG2	1.00	0.008	1.00	2.01
LYS19	HG3	1.00	0.002	1.00	1.47
LYS19	HD2	1.00	0.004	1.00	1.47
LYS19	HE2	1.00	0.008	1.00	0.28
LYS19	H	1.00	0.000	1.00	0.12
LYS20	H	0.97	1.229	0.03	0.00

3.19.4 Detailed Probabilities of LYS19CD:

Overall probability: 0.750

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS19	0.75	0.88

Expected NOESY Contacts

Proton	Expected probability
K19HA	0.98
K19HB2	1.00
K19HB3	1.00
K19HG2	1.00
K19HG3	1.00
K19HD3	1.00
K19HE2	1.00
K19HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS19	HA	0.98	0.010	1.00	0.20
LYS19	HB2	1.00	0.208	0.00	0.00
LYS19	HB3	1.00	0.254	0.00	0.00
LYS19	HG2	1.00	0.005	1.00	0.82
LYS19	HG3	1.00	0.016	1.00	12.64
LYS19	HD2	1.00	0.014	1.00	12.64
LYS19	HE2	1.00	0.005	1.00	0.78
LYS19	H	0.87	0.007	1.00	0.24

3.19.5 Detailed Probabilities of LYS19CE:

Overall probability: 0.967

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS19	0.97	0.86

Expected NOESY Contacts

Proton	Expected probability
K19HB2	0.98
K19HB3	0.99
K19HG2	1.00
K19HG3	1.00
K19HD2	1.00
K19HE3	1.00
K19HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS19	HB2	0.99	0.032	0.80	0.00
LYS19	HB3	0.99	0.014	1.00	0.26
LYS19	HG2	1.00	0.002	1.00	1.02
LYS19	HG3	1.00	0.001	1.00	1.32
LYS19	HD2	1.00	0.001	1.00	1.32
LYS19	HE2	1.00	0.007	1.00	27.21

3.19.6 Detailed Probabilities of LYS19N:

Overall probability: 0.930

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE18	0.84	1.00
LYS19	1.00	1.00
LYS20	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I18HG21	0.98
I18HB	1.00
I18HG12	0.98
I18H	1.00
I18HA	1.00
K19HA	1.00
K19HB2	1.00
K19HB3	1.00
K19HG2	1.00
K19HG3	1.00
K19H	1.00
K20H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE18	HA	1.00	0.005	1.00	-164697.00
ILE18	HB	1.00	0.006	1.00	-1299732.00
ILE18	HG12	0.98	0.047	0.02	0.00
ILE18	HG21	0.98	0.007	1.00	-605560.00
ILE18	H	1.00	0.005	1.00	-655058.00
ILE18	HG13	0.95	0.004	1.00	-605560.00
LYS19	HA	1.00	0.002	1.00	-493250.00
LYS19	HB2	1.00	0.027	1.00	-1299732.00
LYS19	HB3	1.00	0.019	1.00	-1299732.00
LYS19	HG2	1.00	0.003	1.00	-266354.00
LYS19	HG3	1.00	0.002	1.00	-786998.00
LYS19	H	1.00	0.005	1.00	-4537728.00
LYS19	HD2	0.88	0.004	1.00	-786998.00
LYS20	H	1.00	0.002	1.00	-496806.00

3.19.7 Detailed Probabilities of LYS19HA:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE18	0.00	1.00
LYS19	1.00	1.00
LYS20	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I18HA	1.00
K19HB2	1.00
K19HB3	1.00
K19HG2	1.00
K19HG3	1.00
K19HD2	0.98
K19H	1.00
K19HA	1.00
K20HA	1.00
K20H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE18	HA	1.00	0.295	0.00	0.00
LYS19	HA	1.00	0.004	1.00	4.48
LYS19	HB2	1.00	0.005	1.00	0.35
LYS19	HB3	1.00	0.005	1.00	0.35
LYS19	HG2	1.00	0.001	1.00	0.30
LYS19	HG3	1.00	0.014	1.00	0.22
LYS19	HD2	0.98	0.010	1.00	0.20
LYS19	H	1.00	0.002	1.00	-493250.00
LYS20	HA	1.00	0.008	1.00	0.13
LYS20	H	1.00	0.001	1.00	-264583.00

3.19.8 Detailed Probabilities of LYS19HB2:

Overall probability: 0.400

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS19	0.45	1.00
LYS20	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K19HA	1.00
K19HB3	1.00
K19HG2	1.00
K19HG3	1.00
K19HD2	1.00
K19HE2	0.98
K19H	1.00
K19HB2	1.00
K20H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS19	HA	1.00	0.036	0.40	0.00
LYS19	HB2	1.00	0.092	0.00	0.00
LYS19	HB3	1.00	0.602	0.00	0.00
LYS19	HG2	1.00	0.036	0.40	0.00
LYS19	HG3	1.00	0.003	1.00	1.10
LYS19	HD2	1.00	0.208	0.00	0.00
LYS19	HE2	0.98	0.032	0.80	0.00
LYS19	H	1.00	0.027	1.00	-1299732.00
LYS20	H	1.00	0.094	0.00	0.00

3.19.9 Detailed Probabilities of LYS19HB3:

Overall probability: 0.556

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS19	0.63	1.00
LYS20	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K19HA	1.00
K19HB2	1.00
K19HG2	1.00
K19HG3	1.00
K19HD2	1.00
K19HE2	0.99
K19H	1.00
K19HB3	1.00
K20H	1.00

NOESY contacts detailed probability

3.19 LYS(19)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS19	HA	1.00	0.010	1.00	0.71
LYS19	HB2	1.00	0.046	0.00	0.00
LYS19	HB3	1.00	0.648	0.00	0.00
LYS19	HG2	1.00	0.010	1.00	0.36
LYS19	HG3	1.00	0.014	1.00	1.00
LYS19	HD2	1.00	0.254	0.00	0.00
LYS19	HE2	0.99	0.014	1.00	0.26
LYS19	H	1.00	0.019	1.00	-1299732.00
LYS20	H	1.00	0.048	0.00	0.00

3.19.10 Detailed Probabilities of LYS19HG2:

Overall probability: 1.000

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS19	1.00	0.89
LYS20	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K19HA	1.00
K19HB2	1.00
K19HB3	1.00
K19HG3	1.00
K19HD2	1.00
K19HE2	1.00
K19H	1.00
K19HZ2	1.00
K19HG2	1.00
K20H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS19	HA	1.00	0.001	1.00	0.42
LYS19	HB2	1.00	0.014	1.00	0.26
LYS19	HB3	1.00	0.005	1.00	0.34
LYS19	HG2	1.00	0.008	1.00	2.01
LYS19	HG3	1.00	0.003	1.00	1.02
LYS19	HD2	1.00	0.005	1.00	0.82
LYS19	HE2	1.00	0.002	1.00	1.02
LYS19	H	1.00	0.003	1.00	-266354.00
LYS20	H	0.97	0.005	1.00	-102960.00

3.19.11 Detailed Probabilities of LYS19HG3:

Overall probability: 0.778

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS19	0.75	0.89
LYS20	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K19HA	1.00
K19HB2	1.00
K19HB3	1.00
K19HG2	1.00
K19HD2	1.00
K19HE2	1.00
K19H	1.00
K19HZ2	1.00
K19HG3	1.00
K20H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS19	HA	1.00	0.003	1.00	0.54
LYS19	HB2	1.00	0.000	1.00	1.03
LYS19	HB3	1.00	0.410	0.00	0.00
LYS19	HG2	1.00	0.002	1.00	1.47
LYS19	HG3	1.00	0.040	0.00	0.00
LYS19	HD2	1.00	0.016	1.00	12.64
LYS19	HE2	1.00	0.001	1.00	1.32
LYS19	H	1.00	0.002	1.00	-786998.00
LYS20	H	0.96	0.011	1.00	-200228.00

3.19.12 Detailed Probabilities of LYS19HD2:

Overall probability: 0.750

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS19	0.75	0.88

Expected NOESY Contacts

Proton	Expected probability
K19HA	0.98
K19HB2	1.00
K19HB3	1.00
K19HG2	1.00
K19HG3	1.00
K19HD3	1.00
K19HE2	1.00
K19HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS19	HA	0.98	0.005	1.00	0.54
LYS19	HB2	1.00	0.002	1.00	1.03
LYS19	HB3	1.00	0.408	0.00	0.00
LYS19	HG2	1.00	0.004	1.00	1.47
LYS19	HG3	1.00	0.197	0.00	0.00
LYS19	HD2	1.00	0.014	1.00	12.64
LYS19	HE2	1.00	0.001	1.00	1.32
LYS19	H	0.87	0.004	1.00	-786998.00

3.19.13 Detailed Probabilities of LYS19HE2:

Overall probability: 0.859

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS19	0.86	0.86

Expected NOESY Contacts

Proton	Expected probability
K19HB2	0.98
K19HB3	0.99
K19HG2	1.00
K19HG3	1.00
K19HD2	1.00
K19HE3	1.00
K19HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS19	HB2	0.99	0.008	1.00	0.10
LYS19	HB3	0.99	0.136	0.01	0.00
LYS19	HG2	1.00	0.008	1.00	0.28
LYS19	HG3	1.00	0.013	1.00	0.28
LYS19	HD2	1.00	0.005	1.00	0.78
LYS19	HE2	1.00	0.007	1.00	27.21
LYS19	HA	0.76	0.001	1.00	0.10

3.19.14 Detailed Probabilities of LYS19H:

Overall probability: 0.930

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE18	0.80	1.00
LYS19	1.00	1.00
LYS20	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I18HG21	0.98
I18HB	1.00
I18HG12	0.98
I18H	1.00
I18HA	1.00
K19HA	1.00
K19HB2	1.00
K19HB3	1.00
K19HG2	1.00
K19HG3	1.00
K19H	1.00
K20H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE18	HA	1.00	0.010	1.00	0.13
ILE18	HB	1.00	0.011	1.00	0.34
ILE18	HG12	0.98	0.118	0.02	0.00
ILE18	HG21	0.98	0.016	1.00	0.61
ILE18	H	1.00	0.007	1.00	-580792.00
LYS19	HA	1.00	0.009	1.00	0.36
LYS19	HB2	1.00	0.013	1.00	0.26
LYS19	HB3	1.00	0.004	1.00	0.27
LYS19	HG2	1.00	0.000	1.00	0.12
LYS19	HG3	1.00	0.009	1.00	0.20
LYS19	H	1.00	0.005	1.00	-4537728.00
LYS19	HD2	0.88	0.007	1.00	0.24
LYS20	H	1.00	0.007	1.00	-654692.00
LYS20	HA	0.88	0.008	1.00	0.37

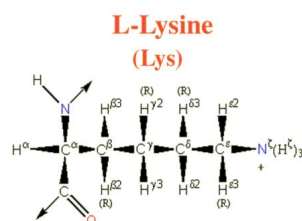


Figure 20: Image from the BMRB

Residue probability: 0.810
Residue probability confidence: 0.931

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.406	176.660	3.133	0.000	0.000
CA 3.20.1	58.539	57.014	3.028	0.692	1.000
CB 3.20.2	31.981	32.981	3.186	0.911	1.000
CG 3.20.3	24.444	24.941	1.956	0.811	0.900
CD 3.20.4	28.780	29.020	2.193	0.875	0.875
CE 3.20.5	41.780	41.893	1.492	0.859	0.857
N 3.20.6	116.284	120.954	4.210	0.867	1.000
NZ	NA	—	—	0.000	0.000
HA 3.20.7	4.087	4.262	0.489	0.818	1.000
HB 3.20.8	1.890	1.774	0.365	0.668	1.000
HG2 3.20.9	1.506	1.358	0.344	0.558	0.900
HG3 3.20.10	1.476	1.343	0.357	0.703	0.900
HD2 3.20.11	1.687	1.614	0.957	1.000	0.875
HD3 3.20.12	1.686	1.595	0.387	1.000	0.875
HE 3.20.13	2.964	2.907	0.230	0.786	0.857
H 3.20.14	7.303	8.185	0.605	0.791	1.000
HZ	NA	—	—	0.000	0.000

3.20.1 Detailed Probabilities of LYS20CA:

Overall probability: 0.692
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS19	1.00	1.00
LYS20	0.66	1.00
GLU21	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K19HA	1.00
K20HB2	1.00
K20HG2	1.00
K20HG3	1.00
K20HD2	0.98
K20HD3	0.98
K20H	1.00
K20HA	1.00
E21HA	1.00
E21H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS19	HA	1.00	0.008	1.00	0.13
LYS19	H	0.88	0.008	1.00	0.37
LYS20	HA	1.00	0.045	0.00	0.00
LYS20	HB2	1.00	0.022	1.00	3.96
LYS20	HG2	1.00	0.067	0.00	0.00
LYS20	HG3	1.00	0.037	0.30	0.00
LYS20	HD2	0.98	0.001	1.00	1.91
LYS20	HD3	0.98	0.000	1.00	1.91
LYS20	H	1.00	0.005	1.00	0.83
LYS20	HE2	0.77	0.002	1.00	0.49
GLU21	HA	1.00	0.079	0.00	0.00
GLU21	H	1.00	0.006	1.00	0.52

3.20.2 Detailed Probabilities of LYS20CB:

Overall probability: 0.911

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS20	0.90	1.00
GLU21	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K20HA	1.00
K20HB3	1.00
K20HG2	1.00
K20HG3	1.00
K20HD2	1.00
K20HD3	1.00
K20HE2	0.98
K20H	1.00
E21H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS20	HA	1.00	0.002	1.00	4.53
LYS20	HB2	1.00	0.014	1.00	53.87
LYS20	HG2	1.00	0.033	0.70	0.00
LYS20	HG3	1.00	0.003	1.00	3.41
LYS20	HD2	1.00	0.004	1.00	5.56
LYS20	HD3	1.00	0.003	1.00	5.56
LYS20	HE2	0.99	0.035	0.50	0.00
LYS20	H	1.00	0.006	1.00	1.38
GLU21	H	1.00	0.026	1.00	0.92

3.20.3 Detailed Probabilities of LYS20CG:

Overall probability: 0.811

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS20	0.79	0.89
GLU21	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K20HA	1.00
K20HB2	1.00
K20HG2	1.00
K20HD2	1.00
K20HD3	1.00
K20HE2	1.00
K20H	1.00
K20HZ2	1.00
K20HG3	1.00
E21H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS20	HA	1.00	0.001	1.00	0.93
LYS20	HB2	1.00	0.002	1.00	2.94
LYS20	HG2	1.00	0.037	0.30	0.00
LYS20	HG3	1.00	0.007	1.00	52.13
LYS20	HD2	1.00	0.005	1.00	6.34
LYS20	HD3	1.00	0.004	1.00	6.34
LYS20	HE2	1.00	0.239	0.00	0.00
LYS20	H	1.00	0.009	1.00	0.26
GLU21	H	0.97	0.026	1.00	0.24

3.20.4 Detailed Probabilities of LYS20CD:

Overall probability: 0.875

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS20	0.88	0.88

Expected NOESY Contacts

Proton	Expected probability
K20HA	0.98
K20HB2	1.00
K20HG2	1.00
K20HG3	1.00
K20HD2	1.00
K20HE2	1.00
K20HZ2	1.00
K20HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS20	HA	0.98	0.004	1.00	1.30
LYS20	HB2	1.00	0.042	0.00	0.00
LYS20	HG2	1.00	0.009	1.00	11.42
LYS20	HG3	1.00	0.021	1.00	11.42
LYS20	HD2	1.00	0.003	1.00	244.35
LYS20	HD3	1.00	0.002	1.00	244.35
LYS20	HE2	1.00	0.018	1.00	6.07
LYS20	H	0.87	0.012	1.00	0.11

3.20.5 Detailed Probabilities of LYS20CE:

Overall probability: 0.859

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS20	0.86	0.86

Expected NOESY Contacts

Proton	Expected probability
K20HB2	0.98
K20HG2	1.00
K20HG3	1.00
K20HD2	1.00
K20HD3	1.00
K20HE3	1.00
K20HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS20	HB2	0.98	0.040	0.02	0.00
LYS20	HG2	1.00	0.014	1.00	3.64
LYS20	HG3	1.00	0.016	1.00	3.64
LYS20	HD2	1.00	0.009	1.00	15.02
LYS20	HD3	1.00	0.010	1.00	15.02
LYS20	HE2	1.00	0.023	1.00	641.65
LYS20	HA	0.76	0.022	1.00	0.98

3.20.6 Detailed Probabilities of LYS20N:

Overall probability: 0.867

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS19	0.71	1.00
LYS20	1.00	1.00
GLU21	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K19HB2	1.00
K19HG3	0.96
K19HB3	1.00
K19HA	1.00
K19HG2	0.97
K19H	1.00
K20HA	1.00
K20HB2	1.00
K20HG2	1.00
K20HG3	1.00
K20H	1.00
E21H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS19	HA	1.00	0.001	1.00	-264583.00
LYS19	HB2	1.00	0.094	0.00	0.00
LYS19	HB3	1.00	0.048	0.00	0.00
LYS19	HG2	0.97	0.005	1.00	-102960.00
LYS19	HG3	0.96	0.011	1.00	-200228.00
LYS19	H	1.00	0.007	1.00	-654692.00
LYS19	HD2	0.56	0.013	1.00	-200228.00
LYS20	HA	1.00	0.004	1.00	-1175133.00
LYS20	HB2	1.00	0.008	1.00	-2913245.00
LYS20	HG2	1.00	0.016	1.00	-474849.00
LYS20	HG3	1.00	0.014	1.00	-474849.00
LYS20	H	1.00	0.003	1.00	-9831361.00
GLU21	H	1.00	0.006	1.00	-1107315.00
GLU21	HA	0.87	0.027	1.00	-348510.00
GLU21	HB2	0.66	0.006	1.00	-163002.00

3.20.7 Detailed Probabilities of LYS20HA:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS19	1.00	1.00
LYS20	0.88	1.00
GLU21	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K19HA	1.00
K20HB2	1.00
K20HG2	1.00
K20HG3	1.00
K20HD2	0.98
K20HD3	0.98
K20H	1.00
K20HA	1.00
E21HA	1.00
E21H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS19	HA	1.00	0.016	1.00	0.06
LYS20	HA	1.00	0.045	0.00	0.00
LYS20	HB2	1.00	0.002	1.00	4.53
LYS20	HG2	1.00	0.003	1.00	1.20
LYS20	HG3	1.00	0.001	1.00	0.93
LYS20	HD2	0.98	0.004	1.00	1.30
LYS20	HD3	0.98	0.004	1.00	1.30
LYS20	H	1.00	0.004	1.00	-1175133.00
LYS20	HE2	0.77	0.022	1.00	0.98
GLU21	HA	1.00	0.595	0.00	0.00
GLU21	H	1.00	0.020	1.00	-1383855.00

3.20.8 Detailed Probabilities of LYS20HB2:

Overall probability: 0.668

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS20	0.63	1.00
GLU21	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K20HA	1.00
K20HB3	1.00
K20HG2	1.00
K20HG3	1.00
K20HD2	1.00
K20HD3	1.00
K20HE2	0.98
K20H	1.00
E21H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS20	HA	1.00	0.022	1.00	3.96
LYS20	HB2	1.00	0.014	1.00	53.87
LYS20	HG2	1.00	0.007	1.00	2.42
LYS20	HG3	1.00	0.002	1.00	2.94
LYS20	HD2	1.00	0.042	0.00	0.00
LYS20	HD3	1.00	0.042	0.00	0.00
LYS20	HE2	0.98	0.040	0.02	0.00
LYS20	H	1.00	0.008	1.00	-2913245.00
GLU21	H	1.00	0.012	1.00	-1317662.00

3.20.9 Detailed Probabilities of LYS20HG2:

Overall probability: 0.558

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS20	0.63	0.89
GLU21	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
K20HA	1.00
K20HB2	1.00
K20HG3	1.00
K20HD2	1.00
K20HD3	1.00
K20HE2	1.00
K20H	1.00
K20HZ2	1.00
K20HG2	1.00
E21H	0.98

NOESY contacts detailed probability

3.20 LYS(20)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS20	HA	1.00	0.067	0.00	0.00
LYS20	HB2	1.00	0.033	0.70	0.00
LYS20	HG2	1.00	0.176	0.00	0.00
LYS20	HG3	1.00	0.037	0.30	0.00
LYS20	HD2	1.00	0.009	1.00	11.42
LYS20	HD3	1.00	0.009	1.00	11.42
LYS20	HE2	1.00	0.014	1.00	3.64
LYS20	H	1.00	0.016	1.00	-474849.00
GLU21	H	0.98	0.042	0.02	0.00

3.20.10 Detailed Probabilities of LYS20HG3:

Overall probability: 0.703

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS20	0.79	0.89
GLU21	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
K20HA	1.00
K20HB2	1.00
K20HG2	1.00
K20HD2	1.00
K20HD3	1.00
K20HE2	1.00
K20H	1.00
K20HZ2	1.00
K20HG3	1.00
E21H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS20	HA	1.00	0.037	0.30	0.00
LYS20	HB2	1.00	0.003	1.00	3.41
LYS20	HG2	1.00	0.206	0.00	0.00
LYS20	HG3	1.00	0.007	1.00	52.13
LYS20	HD2	1.00	0.021	1.00	11.42
LYS20	HD3	1.00	0.021	1.00	11.42
LYS20	HE2	1.00	0.016	1.00	3.64
LYS20	H	1.00	0.014	1.00	-474849.00
GLU21	H	0.97	0.072	0.03	0.00

3.20.11 Detailed Probabilities of LYS20HD2:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS20	1.00	0.88

Expected NOESY Contacts

Proton	Expected probability
K20HA	0.98
K20HB2	1.00
K20HG2	1.00
K20HG3	1.00
K20HD3	1.00
K20HE2	1.00
K20HZ2	1.00
K20HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS20	HA	0.98	0.001	1.00	1.91
LYS20	HB2	1.00	0.004	1.00	5.56
LYS20	HG2	1.00	0.005	1.00	6.34
LYS20	HG3	1.00	0.005	1.00	6.34
LYS20	HD2	1.00	0.003	1.00	244.35
LYS20	HD3	1.00	0.003	1.00	244.35
LYS20	HE2	1.00	0.009	1.00	15.02

3.20.12 Detailed Probabilities of LYS20HD3:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS20	1.00	0.88

Expected NOESY Contacts

Proton	Expected probability
K20HA	0.98
K20HB2	1.00
K20HG2	1.00
K20HG3	1.00
K20HD2	1.00
K20HE2	1.00
K20HZ2	1.00
K20HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS20	HA	0.98	0.000	1.00	1.91
LYS20	HB2	1.00	0.003	1.00	5.56
LYS20	HG2	1.00	0.004	1.00	6.34
LYS20	HG3	1.00	0.004	1.00	6.34
LYS20	HD2	1.00	0.002	1.00	244.35
LYS20	HD3	1.00	0.002	1.00	244.35
LYS20	HE2	1.00	0.010	1.00	15.02

3.20.13 Detailed Probabilities of LYS20HE2:

Overall probability: 0.786

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS20	0.79	0.86

Expected NOESY Contacts

Proton	Expected probability
K20HB2	0.98
K20HG2	1.00
K20HG3	1.00
K20HD2	1.00
K20HD3	1.00
K20HE3	1.00
K20HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS20	HB2	0.99	0.035	0.50	0.00
LYS20	HG2	1.00	0.022	1.00	0.99
LYS20	HG3	1.00	0.239	0.00	0.00
LYS20	HD2	1.00	0.018	1.00	6.07
LYS20	HD3	1.00	0.018	1.00	6.07
LYS20	HE2	1.00	0.023	1.00	641.65
LYS20	HA	0.76	0.002	1.00	0.49

3.20.14 Detailed Probabilities of LYS20H:

Overall probability: 0.791

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS19	0.51	1.00
LYS20	1.00	1.00
GLU21	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K19HB2	1.00
K19HG3	0.96
K19HB3	1.00
K19HA	1.00
K19HG2	0.97
K19H	1.00
K20HA	1.00
K20HB2	1.00
K20HG2	1.00
K20HG3	1.00
K20H	1.00
E21H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS19	HA	1.00	0.007	1.00	0.16
LYS19	HB2	1.00	0.001	1.00	0.15
LYS19	HB3	1.00	0.994	0.00	0.00
LYS19	HG2	0.97	1.229	0.03	0.00
LYS19	HG3	0.96	0.187	0.04	0.00
LYS19	H	1.00	0.002	1.00	-496806.00
LYS20	HA	1.00	0.005	1.00	0.83
LYS20	HB2	1.00	0.006	1.00	1.38
LYS20	HG2	1.00	0.007	1.00	0.21
LYS20	HG3	1.00	0.009	1.00	0.26
LYS20	H	1.00	0.003	1.00	-9831361.00
LYS20	HD2	0.88	0.012	1.00	0.11
LYS20	HD3	0.87	0.012	1.00	0.11
GLU21	H	1.00	0.001	1.00	-688062.00

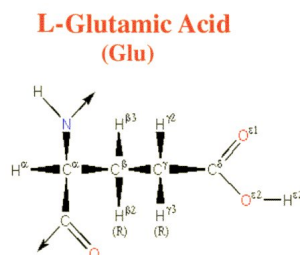
3.21 GLU(21)

Figure 21: Image from the BMRB

Residue probability: 0.627

Residue probability confidence: 0.925

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	179.088	176.942	2.547	0.000	0.000
CA 3.21.1	58.894	57.442	3.837	0.222	1.000
CB 3.21.2	29.434	30.185	4.018	0.571	0.875
CG 3.21.3	35.314	36.085	1.533	1.000	0.875
N 3.21.4	118.488	120.574	4.837	0.754	1.000
HA 3.21.5	3.963	4.245	0.429	0.500	1.000
HB2 3.21.6	2.116	2.021	0.233	0.571	0.875
HB3 3.21.7	1.973	1.994	0.244	0.500	0.875
HG2 3.21.8	2.106	2.258	0.226	0.574	0.875
HG3 3.21.9	2.104	2.233	0.232	0.577	0.875
H 3.21.10	7.665	8.332	0.601	1.000	1.000
HE2	NA	—	—	0.000	0.000

3.21.1 Detailed Probabilities of GLU21CA:

Overall probability: 0.222

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS20	0.00	1.00
GLU21	0.17	1.00
VAL22	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K20HA	1.00
E21HB2	1.00
E21HB3	1.00
E21HG2	1.00
E21HG3	1.00
E21H	1.00
E21HA	1.00
V22H	1.00
V22HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS20	HA	1.00	0.595	0.00	0.00
GLU21	HA	1.00	0.719	0.00	0.00
GLU21	HB2	1.00	0.838	0.00	0.00
GLU21	HB3	1.00	0.695	0.00	0.00
GLU21	HG2	1.00	0.828	0.00	0.00
GLU21	HG3	1.00	0.826	0.00	0.00
GLU21	H	1.00	0.008	1.00	0.87
VAL22	HA	1.00	0.550	0.00	0.00
VAL22	H	1.00	0.020	1.00	0.21

3.21.2 Detailed Probabilities of GLU21CB:

Overall probability: 0.571

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU21	0.67	0.86
VAL22	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E21HA	1.00
E21HB3	1.00
E21HG2	1.00
E21HG3	1.00
E21H	1.00
E21HE2	1.00
E21HB2	1.00
V22H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU21	HA	1.00	0.073	0.00	0.00
GLU21	HB2	1.00	0.023	1.00	35.26
GLU21	HB3	1.00	0.112	0.00	0.00
GLU21	HG2	1.00	0.013	1.00	35.26
GLU21	HG3	1.00	0.011	1.00	35.26
GLU21	H	1.00	0.005	1.00	0.88
VAL22	H	1.00	0.066	0.00	0.00

3.21.3 Detailed Probabilities of GLU21CG:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU21	1.00	0.86
VAL22	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E21HA	1.00
E21HB2	1.00
E21HB3	1.00
E21HG3	1.00
E21H	1.00
E21HE2	1.00
E21HG2	1.00
V22H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU21	HA	1.00	0.003	1.00	0.60
GLU21	HB2	1.00	0.007	1.00	17.61
GLU21	HB3	1.00	0.004	1.00	2.24
GLU21	HG2	1.00	0.003	1.00	17.61
GLU21	HG3	1.00	0.005	1.00	17.61
GLU21	H	1.00	0.007	1.00	0.67
VAL22	H	0.98	0.008	1.00	0.28

3.21.4 Detailed Probabilities of GLU21N:

Overall probability: 0.754

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS20	0.61	1.00
GLU21	0.83	1.00
VAL22	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K20HG3	0.97
K20HB2	1.00
K20HA	1.00
K20H	1.00
K20HG2	0.98
E21HA	1.00
E21HB2	1.00
E21HB3	1.00
E21HG2	1.00
E21HG3	1.00
E21H	1.00
V22H	1.00

NOESY contacts detailed probability

3.21 GLU(21)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS20	HA	1.00	0.020	1.00	-1383855.00
LYS20	HB2	1.00	0.012	1.00	-1317662.00
LYS20	HG2	0.98	0.042	0.02	0.00
LYS20	HG3	0.97	0.072	0.03	0.00
LYS20	H	1.00	0.001	1.00	-688062.00
GLU21	HA	1.00	0.004	1.00	-703970.00
GLU21	HB2	1.00	0.003	1.00	-1493546.00
GLU21	HB3	1.00	0.071	0.00	0.00
GLU21	HG2	1.00	0.007	1.00	-1493546.00
GLU21	HG3	1.00	0.009	1.00	-1493546.00
GLU21	H	1.00	0.021	1.00	-19107776.00
VAL22	H	1.00	0.014	1.00	-355031.00

3.21.5 Detailed Probabilities of GLU21HA:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS20	0.50	1.00
GLU21	0.67	1.00
VAL22	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K20HA	1.00
E21HB2	1.00
E21HB3	1.00
E21HG2	1.00
E21HG3	1.00
E21H	1.00
E21HA	1.00
V22H	1.00
V22HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS20	HA	1.00	0.079	0.00	0.00
LYS20	H	0.87	0.027	1.00	-348510.00
GLU21	HA	1.00	0.719	0.00	0.00
GLU21	HB2	1.00	0.073	0.00	0.00
GLU21	HB3	1.00	0.005	1.00	0.51
GLU21	HG2	1.00	0.003	1.00	0.60
GLU21	HG3	1.00	0.003	1.00	0.60
GLU21	H	1.00	0.004	1.00	-703970.00
VAL22	HA	1.00	0.158	0.00	0.00
VAL22	H	1.00	3.112	0.00	0.00

3.21.6 Detailed Probabilities of GLU21HB2:

Overall probability: 0.571

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU21	0.67	0.86
VAL22	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E21HA	1.00
E21HB3	1.00
E21HG2	1.00
E21HG3	1.00
E21H	1.00
E21HE2	1.00
E21HB2	1.00
V22H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU21	HA	1.00	0.838	0.00	0.00
GLU21	HB2	1.00	0.023	1.00	35.26
GLU21	HB3	1.00	0.713	0.00	0.00
GLU21	HG2	1.00	0.007	1.00	17.61
GLU21	HG3	1.00	0.007	1.00	17.61
GLU21	H	1.00	0.003	1.00	-1493546.00
VAL22	H	1.00	1.265	0.00	0.00

3.21.7 Detailed Probabilities of GLU21HB3:

Overall probability: 0.500

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU21	0.50	0.86
VAL22	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E21HA	1.00
E21HB2	1.00
E21HG2	1.00
E21HG3	1.00
E21H	1.00
E21HE2	1.00
E21HB3	1.00
V22H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU21	HA	1.00	0.695	0.00	0.00
GLU21	HB2	1.00	0.112	0.00	0.00
GLU21	HB3	1.00	0.015	1.00	11.43
GLU21	HG2	1.00	0.004	1.00	2.24
GLU21	HG3	1.00	0.004	1.00	2.24
GLU21	H	1.00	0.071	0.00	0.00
VAL22	H	1.00	1.122	0.00	0.00
VAL22	HA	0.84	0.028	1.00	0.94

3.21.8 Detailed Probabilities of GLU21HG2:

Overall probability: 0.574

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU21	0.67	0.86
VAL22	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
E21HA	1.00
E21HB2	1.00
E21HB3	1.00
E21HG3	1.00
E21H	1.00
E21HE2	1.00
E21HG2	1.00
V22H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU21	HA	1.00	0.828	0.00	0.00
GLU21	HB2	1.00	0.013	1.00	35.26
GLU21	HB3	1.00	0.703	0.00	0.00
GLU21	HG2	1.00	0.003	1.00	17.61
GLU21	HG3	1.00	0.003	1.00	17.61
GLU21	H	1.00	0.007	1.00	-1493546.00
VAL22	H	0.98	1.255	0.02	0.00

3.21.9 Detailed Probabilities of GLU21HG3:

Overall probability: 0.577

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU21	0.67	0.86
VAL22	0.04	1.00

Expected NOESY Contacts

Proton	Expected probability
E21HA	1.00
E21HB2	1.00
E21HB3	1.00
E21HG2	1.00
E21H	1.00
E21HE2	1.00
E21HG3	1.00
V22H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU21	HA	1.00	0.826	0.00	0.00
GLU21	HB2	1.00	0.011	1.00	35.26
GLU21	HB3	1.00	0.701	0.00	0.00
GLU21	HG2	1.00	0.005	1.00	17.61
GLU21	HG3	1.00	0.005	1.00	17.61
GLU21	H	1.00	0.009	1.00	-1493546.00
VAL22	H	0.96	1.253	0.04	0.00

3.21.10 Detailed Probabilities of GLU21H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS20	1.00	1.00
GLU21	1.00	1.00
VAL22	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K20HG3	0.97
K20HB2	1.00
K20HA	1.00
K20H	1.00
K20HG2	0.98
E21HA	1.00
E21HB2	1.00
E21HB3	1.00
E21HG2	1.00
E21HG3	1.00
E21H	1.00
V22H	1.00

NOESY contacts detailed probability

3.21 GLU(21)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS20	HA	1.00	0.006	1.00	0.52
LYS20	HB2	1.00	0.026	1.00	0.92
LYS20	HG2	0.98	0.026	1.00	0.24
LYS20	HG3	0.97	0.026	1.00	0.24
LYS20	H	1.00	0.006	1.00	-1107315.00
GLU21	HA	1.00	0.008	1.00	0.87
GLU21	HB2	1.00	0.005	1.00	0.88
GLU21	HB3	1.00	0.010	1.00	0.60
GLU21	HG2	1.00	0.007	1.00	0.67
GLU21	HG3	1.00	0.007	1.00	0.67
GLU21	H	1.00	0.021	1.00	-19107776.00
VAL22	H	1.00	0.008	1.00	-78904.00

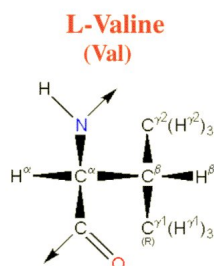
3.22 VAL(22)

Figure 22: Image from the BMRB

Residue probability: 0.827

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 3.22.1	62.799	62.613	4.828	0.857	1.000
CB 3.22.2	29.829	32.918	4.591	0.800	1.000
CG1 3.22.3	20.110	21.563	2.746	1.000	1.000
CG2 3.22.4	19.942	21.368	2.801	1.000	1.000
N 3.22.5	109.032	121.057	5.832	0.369	1.000
HA 3.22.6	4.132	4.178	0.599	0.714	1.000
HB 3.22.7	1.984	1.980	0.322	0.800	1.000
HG1 3.22.8	0.638	0.816	0.264	1.000	1.000
HG2 3.22.9	0.854	0.803	0.504	1.000	1.000
H 3.22.10	8.037	8.311	0.669	0.727	1.000

3.22.1 Detailed Probabilities of VAL22CA:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU21	0.50	1.00
VAL22	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E21HA	1.00
V22HG11	1.00
V22HG21	1.00
V22H	1.00
V22HB	1.00
V22HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU21	HA	1.00	0.158	0.00	0.00
GLU21	HB3	0.84	0.028	1.00	0.94
VAL22	HA	1.00	0.011	1.00	15.35
VAL22	HB	1.00	0.017	1.00	0.94
VAL22	HG11	1.00	0.007	1.00	1.15
VAL22	HG21	1.00	0.001	1.00	0.48
VAL22	H	1.00	0.005	1.00	0.84

3.22.2 Detailed Probabilities of VAL22CB:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL22	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
V22HA	1.00
V22HG11	1.00
V22HG21	1.00
V22H	1.00
V22HB	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL22	HA	1.00	0.012	1.00	0.99
VAL22	HB	1.00	0.026	1.00	11.43
VAL22	HG11	1.00	0.010	1.00	0.84
VAL22	HG21	1.00	0.001	1.00	0.75
VAL22	H	1.00	0.362	0.00	0.00

3.22.3 Detailed Probabilities of VAL22CG1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL22	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V22HA	1.00
V22HG12	1.00
V22HG21	1.00
V22H	1.00
V22HB	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL22	HA	1.00	0.003	1.00	1.12
VAL22	HB	1.00	0.008	1.00	1.55
VAL22	HG11	1.00	0.005	1.00	30.56
VAL22	HG21	1.00	0.005	1.00	2.82
VAL22	H	1.00	0.012	1.00	0.56

3.22.4 Detailed Probabilities of VAL22CG2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL22	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V22HA	1.00
V22HG11	1.00
V22HG22	1.00
V22H	1.00
V22HB	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL22	HA	1.00	0.007	1.00	0.43
VAL22	HB	1.00	0.008	1.00	0.61
VAL22	HG11	1.00	0.008	1.00	2.02
VAL22	HG21	1.00	0.010	1.00	33.98
VAL22	H	1.00	0.012	1.00	0.55

3.22.5 Detailed Probabilities of VAL22N:

Overall probability: 0.369

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU21	0.18	1.00
VAL22	0.60	1.00

Expected NOESY Contacts

Proton	Expected probability
E21HG2	0.98
E21HA	1.00
E21HB2	1.00
E21HG3	0.96
E21HB3	1.00
E21H	1.00
V22HA	1.00
V22HG11	1.00
V22HG21	1.00
V22HB	1.00
V22H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU21	HA	1.00	3.112	0.00	0.00
GLU21	HB2	1.00	1.265	0.00	0.00
GLU21	HB3	1.00	1.122	0.00	0.00
GLU21	HG2	0.98	1.255	0.02	0.00
GLU21	HG3	0.96	1.253	0.04	0.00
GLU21	H	1.00	0.008	1.00	-78904.00
VAL22	HA	1.00	3.281	0.00	0.00
VAL22	HB	1.00	1.133	0.00	0.00
VAL22	HG11	1.00	0.008	1.00	-118015.00
VAL22	HG21	1.00	0.003	1.00	-89798.00
VAL22	H	1.00	0.011	1.00	-242366.00

3.22.6 Detailed Probabilities of VAL22HA:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU21	0.50	1.00
VAL22	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
E21HA	1.00
V22HG11	1.00
V22HG21	1.00
V22H	1.00
V22HB	1.00
V22HA	1.00

NOESY contacts detailed probability

3.22 VAL(22)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU21	HA	1.00	0.550	0.00	0.00
GLU21	HB3	0.84	0.012	1.00	0.99
VAL22	HA	1.00	0.011	1.00	15.35
VAL22	HB	1.00	0.012	1.00	0.99
VAL22	HG11	1.00	0.003	1.00	1.12
VAL22	HG21	1.00	0.007	1.00	0.43
VAL22	H	1.00	3.281	0.00	0.00

3.22.7 Detailed Probabilities of VAL22HB:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL22	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
V22HA	1.00
V22HG11	1.00
V22HG21	1.00
V22H	1.00
V22HB	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL22	HA	1.00	0.017	1.00	0.94
VAL22	HB	1.00	0.026	1.00	11.43
VAL22	HG11	1.00	0.008	1.00	1.55
VAL22	HG21	1.00	0.008	1.00	0.61
VAL22	H	1.00	1.133	0.00	0.00

3.22.8 Detailed Probabilities of VAL22HG11:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL22	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V22HA	1.00
V22HG12	1.00
V22HG21	1.00
V22H	1.00
V22HB	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL22	HA	1.00	0.007	1.00	1.15
VAL22	HB	1.00	0.010	1.00	0.84
VAL22	HG11	1.00	0.005	1.00	30.56
VAL22	HG21	1.00	0.008	1.00	2.02
VAL22	H	1.00	0.008	1.00	-118015.00

3.22.9 Detailed Probabilities of VAL22HG21:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL22	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V22HA	1.00
V22HG11	1.00
V22HG22	1.00
V22H	1.00
V22HB	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL22	HA	1.00	0.001	1.00	0.48
VAL22	HB	1.00	0.001	1.00	0.75
VAL22	HG11	1.00	0.005	1.00	2.82
VAL22	HG21	1.00	0.010	1.00	33.98
VAL22	H	1.00	0.003	1.00	-89798.00

3.22.10 Detailed Probabilities of VAL22H:

Overall probability: 0.727

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU21	0.67	1.00
VAL22	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
E21HG2	0.98
E21HA	1.00
E21HB2	1.00
E21HG3	0.96
E21HB3	1.00
E21H	1.00
V22HA	1.00
V22HG11	1.00
V22HG21	1.00
V22HB	1.00
V22H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU21	HA	1.00	0.020	1.00	0.21
GLU21	HB2	1.00	0.066	0.00	0.00
GLU21	HB3	1.00	0.362	0.00	0.00
GLU21	HG2	0.98	0.008	1.00	0.28
GLU21	HG3	0.96	0.008	1.00	0.28
GLU21	H	1.00	0.014	1.00	-355031.00
VAL22	HA	1.00	0.005	1.00	0.84
VAL22	HB	1.00	0.362	0.00	0.00
VAL22	HG11	1.00	0.012	1.00	0.56
VAL22	HG21	1.00	0.012	1.00	0.55
VAL22	H	1.00	0.011	1.00	-242366.00

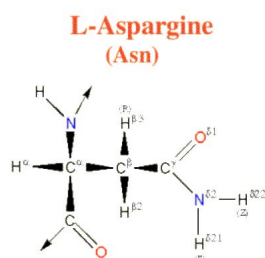
3.23 NA(23)**3.24 ASN(24)**

Figure 23: Image from the BMRB

Residue probability: 0.971

Residue probability confidence: 0.766

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	NA	—	—	0.000	0.000
CA 3.24.1	58.808	53.674	5.429	0.800	0.714
CB 3.24.2	38.171	38.785	5.449	1.000	0.667
N	NA	—	—	0.000	0.000
ND2 3.24.3	112.830	112.932	14.355	1.000	0.800
HA 3.24.4	4.717	4.658	0.371	1.000	0.714
HB 3.24.5	2.967	2.800	0.341	1.000	0.667
H	NA	—	—	0.000	0.000
HD21 3.24.6	7.693	7.343	1.188	1.000	0.800
HD22 3.24.7	6.941	7.145	1.184	1.000	1.000

3.24.1 Detailed Probabilities of ASN24CA:

Overall probability: 0.800

Overall confidence: 0.714

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN24	1.00	0.80
GLN25	0.00	0.50

Expected NOESY Contacts

Proton	Expected probability
N24HB2	1.00
N24H	1.00
N24HD21	1.00
N24HD22	1.00
N24HA	1.00
Q25HA	1.00
Q25H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN24	HA	1.00	0.028	1.00	0.48
ASN24	HB2	1.00	0.023	1.00	0.49
ASN24	HD21	1.00	0.029	1.00	0.38
ASN24	HD22	1.00	0.019	1.00	0.56
GLN25	HA	1.00	0.043	0.00	0.00

3.24.2 Detailed Probabilities of ASN24CB:

Overall probability: 1.000

Overall confidence: 0.667

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN24	1.00	0.80
GLN25	0.00	0.00

Expected NOESY Contacts

Proton	Expected probability
N24HA	1.00
N24HB3	1.00
N24H	1.00
N24HD21	1.00
N24HD22	1.00
Q25H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN24	HA	1.00	0.003	1.00	1.36
ASN24	HB2	1.00	0.001	1.00	27.91
ASN24	HD21	1.00	0.007	1.00	0.66
ASN24	HD22	1.00	0.007	1.00	0.31

3.24.3 Detailed Probabilities of ASN24ND2:

Overall probability: 1.000

Overall confidence: 0.800

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN24	1.00	0.80

Expected NOESY Contacts

Proton	Expected probability
N24HA	1.00
N24HB2	1.00
N24H	0.98
N24HD22	1.00
N24HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN24	HA	1.00	0.000	1.00	-147005.00
ASN24	HB2	1.00	0.002	1.00	-1175436.00
ASN24	HD21	1.00	0.006	1.00	-16235739.00
ASN24	HD22	1.00	0.011	1.00	-12628121.00

3.24.4 Detailed Probabilities of ASN24HA:

Overall probability: 1.000

Overall confidence: 0.714

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN24	1.00	0.80
GLN25	0.00	0.50

Expected NOESY Contacts

Proton	Expected probability
N24HB2	1.00
N24H	1.00
N24HD21	1.00
N24HD22	1.00
N24HA	1.00
Q25HA	1.00
Q25H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN24	HA	1.00	0.028	1.00	0.48
ASN24	HB2	1.00	0.003	1.00	1.36
ASN24	HD21	1.00	0.000	1.00	-147005.00
ASN24	HD22	1.00	0.005	1.00	-102835.00

3.24.5 Detailed Probabilities of ASN24HB2:

Overall probability: 1.000

Overall confidence: 0.667

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN24	1.00	0.80
GLN25	0.00	0.00

Expected NOESY Contacts

Proton	Expected probability
N24HA	1.00
N24HB3	1.00
N24H	1.00
N24HD21	1.00
N24HD22	1.00
Q25H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN24	HA	1.00	0.023	1.00	0.49
ASN24	HB2	1.00	0.001	1.00	27.91
ASN24	HD21	1.00	0.002	1.00	-1175436.00
ASN24	HD22	1.00	0.003	1.00	-724161.00

3.24.6 Detailed Probabilities of ASN24HD21:

Overall probability: 1.000

Overall confidence: 0.800

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN24	1.00	0.80

Expected NOESY Contacts

Proton	Expected probability
N24HA	1.00
N24HB2	1.00
N24H	0.98
N24HD22	1.00
N24HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN24	HA	1.00	0.029	1.00	0.38
ASN24	HB2	1.00	0.007	1.00	0.66
ASN24	HD21	1.00	0.006	1.00	-16235739.00
ASN24	HD22	1.00	0.006	1.00	-13752279.00

3.24.7 Detailed Probabilities of ASN24HD22:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN24	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N24HA	1.00
N24HB2	1.00
N24HD21	1.00
N24HD22	1.00

NOESY contacts detailed probability					
Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN24	HA	1.00	0.019	1.00	0.56
ASN24	HB2	1.00	0.007	1.00	0.31
ASN24	HD21	1.00	0.011	1.00	-12628121.00
ASN24	HD22	1.00	0.011	1.00	-18588282.00

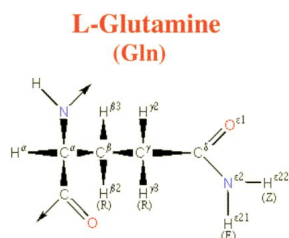


Figure 24: Image from the BMRB

Residue probability: 0.757
Residue probability confidence: 0.919

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	175.692	176.405	1.998	0.000	0.000
CA	NA	—	—	0.000	0.000
CB 3.25.1	29.018	29.436	2.799	0.778	0.889
CG 3.25.2	33.393	33.781	1.871	1.000	0.875
N	NA	—	—	0.000	0.000
NE2 3.25.3	112.873	111.924	2.434	0.714	1.000
HA 3.25.4	4.646	4.265	0.455	0.556	0.900
HB2 3.25.5	2.021	2.047	0.290	0.571	0.889
HB3 3.25.6	2.815	2.012	0.313	0.571	0.889
HG2 3.25.7	2.383	2.308	0.289	0.717	0.875
HG3 3.25.8	2.518	2.284	0.313	0.833	0.875
H	NA	—	—	0.000	0.000
HE21 3.25.9	7.563	7.217	0.496	1.000	1.000
HE22 3.25.10	6.876	7.041	0.463	0.833	1.000

3.25.1 Detailed Probabilities of GLN25CB:

Overall probability: 0.778
Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN25	0.86	0.88
GLY26	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
Q25HA	1.00
Q25HB2	1.00
Q25HG2	1.00
Q25HG3	1.00
Q25H	1.00
Q25HE21	1.00
Q25HE22	1.00
Q25HB3	1.00
G26H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN25	HA	1.00	0.001	1.00	0.39
GLN25	HB2	1.00	0.013	1.00	1.10
GLN25	HB3	1.00	0.001	1.00	1.48
GLN25	HG2	1.00	0.005	1.00	0.32
GLN25	HG3	1.00	0.000	1.00	0.39
GLN25	HE21	1.00	0.003	1.00	0.18
GLN25	HE22	1.00	0.093	0.00	0.00
GLY26	H	1.00	0.460	0.00	0.00
GLY26	HA3	0.72	0.008	1.00	0.10

3.25.2 Detailed Probabilities of GLN25CG:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN25	1.00	0.88

Expected NOESY Contacts

Proton	Expected probability
Q25HA	1.00
Q25HB2	1.00
Q25HB3	1.00
Q25HG2	1.00
Q25H	1.00
Q25HE21	1.00
Q25HE22	1.00
Q25HG3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN25	HA	1.00	0.001	1.00	0.32
GLN25	HB2	1.00	0.011	1.00	0.68
GLN25	HB3	1.00	0.002	1.00	0.55
GLN25	HG2	1.00	0.023	1.00	10.45
GLN25	HG3	1.00	0.006	1.00	28.96
GLN25	HE21	1.00	0.004	1.00	0.46
GLN25	HE22	1.00	0.003	1.00	0.16

3.25.3 Detailed Probabilities of GLN25NE2:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN25	0.71	1.00

Expected NOESY Contacts

Proton	Expected probability
Q25HB2	1.00
Q25HB3	1.00
Q25HG2	1.00
Q25HG3	1.00
Q25HE22	1.00
Q25HE21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN25	HB2	1.00	0.186	0.00	0.00
GLN25	HB3	1.00	0.152	0.00	0.00
GLN25	HG2	1.00	0.004	1.00	-564667.00
GLN25	HG3	1.00	0.006	1.00	-325089.00
GLN25	HE21	1.00	0.004	1.00	-16197423.00
GLN25	HE22	1.00	0.002	1.00	-12009423.00
GLN25	HA	0.94	0.001	1.00	-92692.00

3.25.4 Detailed Probabilities of GLN25HA:

Overall probability: 0.556

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN24	0.00	1.00
GLN25	0.80	0.83
GLY26	0.33	1.00

Expected NOESY Contacts

Proton	Expected probability
N24HA	1.00
Q25HB2	1.00
Q25HB3	1.00
Q25HG2	1.00
Q25HG3	1.00
Q25H	1.00
Q25HA	1.00
G26H	1.00
G26HA2	1.00
G26HA3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN24	HA	1.00	0.043	0.00	0.00
GLN25	HB2	1.00	0.118	0.00	0.00
GLN25	HB3	1.00	0.001	1.00	0.39
GLN25	HG2	1.00	0.005	1.00	0.61
GLN25	HG3	1.00	0.001	1.00	0.32
GLN25	HE21	0.94	0.001	1.00	-92692.00
GLY26	HA2	1.00	0.002	1.00	0.06
GLY26	HA3	1.00	0.138	0.00	0.00
GLY26	H	1.00	0.526	0.00	0.00

3.25.5 Detailed Probabilities of GLN25HB2:

Overall probability: 0.571

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN25	0.67	0.88
GLY26	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q25HA	1.00
Q25HB3	1.00
Q25HG2	1.00
Q25HG3	1.00
Q25H	1.00
Q25HE21	1.00
Q25HE22	1.00
Q25HB2	1.00
G26H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN25	HB2	1.00	0.020	1.00	52.03
GLN25	HB3	1.00	0.013	1.00	1.10
GLN25	HG2	1.00	0.019	1.00	2.35
GLN25	HG3	1.00	0.011	1.00	0.68
GLN25	HE21	1.00	0.186	0.00	0.00
GLN25	HE22	1.00	0.070	0.00	0.00
GLY26	H	1.00	1.759	0.00	0.00

3.25.6 Detailed Probabilities of GLN25HB3:

Overall probability: 0.571

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN25	0.67	0.88
GLY26	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q25HA	1.00
Q25HB2	1.00
Q25HG2	1.00
Q25HG3	1.00
Q25H	1.00
Q25HE21	1.00
Q25HE22	1.00
Q25HB3	1.00
G26H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN25	HB2	1.00	0.005	1.00	1.12
GLN25	HB3	1.00	0.001	1.00	1.48
GLN25	HG2	1.00	0.006	1.00	0.43
GLN25	HG3	1.00	0.002	1.00	0.55
GLN25	HE21	1.00	0.152	0.00	0.00
GLN25	HE22	1.00	0.147	0.00	0.00
GLY26	H	1.00	0.965	0.00	0.00

3.25.7 Detailed Probabilities of GLN25HG2:

Overall probability: 0.717

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN25	0.72	0.88

Expected NOESY Contacts

Proton	Expected probability
Q25HA	1.00
Q25HB2	1.00
Q25HB3	1.00
Q25HG3	1.00
Q25H	1.00
Q25HE21	1.00
Q25HE22	1.00
Q25HG2	1.00

NOESY contacts detailed probability

3.25 GLN(25)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN25	HB2	1.00	0.048	0.00	0.00
GLN25	HB3	1.00	0.005	1.00	0.32
GLN25	HG2	1.00	0.033	0.70	0.00
GLN25	HG3	1.00	0.023	1.00	10.45
GLN25	HE21	1.00	0.004	1.00	-564667.00
GLN25	HE22	1.00	0.034	0.60	0.00

3.25.8 Detailed Probabilities of GLN25HG3:

Overall probability: 0.833

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN25	0.83	0.88

Expected NOESY Contacts

Proton	Expected probability
Q25HA	1.00
Q25HB2	1.00
Q25HB3	1.00
Q25HG2	1.00
Q25H	1.00
Q25HE21	1.00
Q25HE22	1.00
Q25HG3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN25	HB2	1.00	0.130	0.00	0.00
GLN25	HB3	1.00	0.000	1.00	0.39
GLN25	HG2	1.00	0.002	1.00	10.18
GLN25	HG3	1.00	0.006	1.00	28.96
GLN25	HE21	1.00	0.006	1.00	-325089.00
GLN25	HE22	1.00	0.007	1.00	-203111.00

3.25.9 Detailed Probabilities of GLN25HE21:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN25	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q25HB2	1.00
Q25HB3	1.00
Q25HG2	1.00
Q25HG3	1.00
Q25HE22	1.00
Q25HE21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN25	HB2	1.00	0.027	1.00	0.57
GLN25	HB3	1.00	0.003	1.00	0.18
GLN25	HG2	1.00	0.003	1.00	0.67
GLN25	HG3	1.00	0.004	1.00	0.46
GLN25	HE21	1.00	0.004	1.00	-16197423.00
GLN25	HE22	1.00	0.006	1.00	-12602244.00

3.25.10 Detailed Probabilities of GLN25HE22:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN25	0.83	1.00

Expected NOESY Contacts

Proton	Expected probability
Q25HB2	1.00
Q25HB3	1.00
Q25HG2	1.00
Q25HG3	1.00
Q25HE21	1.00
Q25HE22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN25	HB2	1.00	0.000	1.00	0.09
GLN25	HB3	1.00	0.093	0.00	0.00
GLN25	HG2	1.00	0.020	1.00	0.45
GLN25	HG3	1.00	0.003	1.00	0.16
GLN25	HE21	1.00	0.002	1.00	-12009423.00
GLN25	HE22	1.00	0.016	1.00	-31513908.00

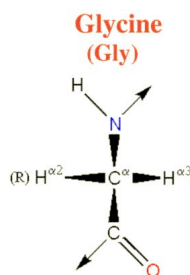
3.26 GLY(26)

Figure 25: Image from the BMRB

Residue probability: 0.632

Residue probability confidence: 0.950

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.382	173.872	2.493	0.000	0.000
CA 3.26.1	45.957	45.581	4.381	0.833	1.000
N 3.26.2	106.368	109.752	5.331	0.429	0.875
HA2 3.26.3	3.815	3.967	0.380	0.800	1.000
HA3 3.26.4	4.126	3.897	0.390	0.600	1.000
H 3.26.5	8.020	8.343	0.939	0.500	0.875

3.26.1 Detailed Probabilities of GLY26CA:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN25	1.00	1.00
GLY26	1.00	1.00
TYR27	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
Q25HA	1.00
G26HA3	1.00
G26H	1.00
G26HA2	1.00
Y27HA	1.00
Y27H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN25	HA	1.00	0.002	1.00	0.06
GLY26	HA2	1.00	0.011	1.00	4.21
GLY26	HA3	1.00	0.002	1.00	2.31
GLY26	H	1.00	0.004	1.00	0.34
TYR27	HA	1.00	0.018	1.00	0.05
TYR27	H	1.00	0.082	0.00	0.00

3.26.2 Detailed Probabilities of GLY26N:

Overall probability: 0.429

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN25	0.00	0.75
GLY26	1.00	1.00
TYR27	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q25HB3	1.00
Q25H	1.00
Q25HA	1.00
Q25HB2	1.00
G26HA2	1.00
G26HA3	1.00
G26H	1.00
Y27H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN25	HA	1.00	0.526	0.00	0.00
GLN25	HB2	1.00	1.759	0.00	0.00
GLN25	HB3	1.00	0.965	0.00	0.00
GLY26	HA2	1.00	0.007	1.00	-184166.00
GLY26	HA3	1.00	0.006	1.00	-135791.00
GLY26	H	1.00	0.008	1.00	-464503.00
TYR27	H	1.00	0.183	0.00	0.00

3.26.3 Detailed Probabilities of GLY26HA2:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN25	0.00	1.00
GLY26	1.00	1.00
TYR27	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
Q25HA	1.00
G26HA3	1.00
G26H	1.00
G26HA2	1.00
Y27HA	1.00
Y27H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLY26	HA2	1.00	0.011	1.00	4.21
GLY26	HA3	1.00	0.006	1.00	2.29
GLY26	H	1.00	0.007	1.00	-184166.00
TYR27	HA	1.00	0.441	0.00	0.00
TYR27	H	1.00	0.022	1.00	-98922.00

3.26.4 Detailed Probabilities of GLY26HA3:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN25	NaN	1.00
GLY26	1.00	1.00
TYR27	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q25HA	1.00
G26HA2	1.00
G26H	1.00
G26HA3	1.00
Y27HA	1.00
Y27H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLY26	HA2	1.00	0.002	1.00	2.31
GLY26	HA3	1.00	0.004	1.00	2.39
GLY26	H	1.00	0.006	1.00	-135791.00
TYR27	HA	1.00	0.309	0.00	0.00
TYR27	H	1.00	0.289	0.00	0.00

3.26.5 Detailed Probabilities of GLY26H:

Overall probability: 0.500

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN25	0.00	0.75
GLY26	1.00	1.00
TYR27	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q25HB3	1.00
Q25H	1.00
Q25HA	1.00
Q25HB2	1.00
G26HA2	1.00
G26HA3	1.00
G26H	1.00
Y27H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN25	HB2	1.00	0.076	0.00	0.00
GLN25	HB3	1.00	0.460	0.00	0.00
GLY26	HA2	1.00	0.004	1.00	0.34
GLY26	HA3	1.00	0.000	1.00	0.31
GLY26	H	1.00	0.008	1.00	-464503.00
TYR27	H	1.00	0.317	0.00	0.00

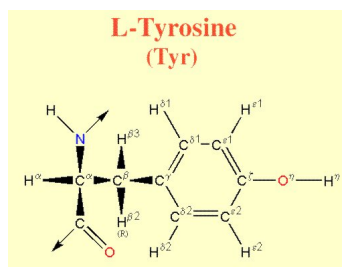


Figure 26: Image from the BMRB

Residue probability: 0.856
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.528	175.405	2.122	0.000	0.000
CA 3.27.1	58.054	58.279	6.333	0.727	1.000
CB 3.27.2	39.005	39.527	6.280	0.875	1.000
CD1 3.27.3	132.650	132.994	20.285	1.000	1.000
CD2 3.27.4	132.816	133.192	23.179	1.000	1.000
CE1 3.27.5	117.793	117.867	2.496	1.000	1.000
CE2 3.27.6	117.910	117.793	3.050	1.000	1.000
N 3.27.7	119.082	120.136	8.494	0.500	1.000
HA 3.27.8	4.433	4.610	0.592	0.700	1.000
HB2 3.27.9	2.663	2.886	0.452	0.800	1.000
HB3 3.27.10	2.372	2.808	0.478	0.900	1.000
HD1 3.27.11	6.787	6.912	0.327	1.000	1.000
HD2 3.27.12	6.787	6.905	0.356	1.000	1.000
HE1 3.27.13	6.586	6.692	0.243	1.000	1.000
HE2 3.27.14	6.586	6.690	0.252	0.834	1.000
H 3.27.15	7.845	8.326	0.740	0.500	1.000
HH	NA	—	—	0.000	0.000

3.27.1 Detailed Probabilities of TYR27CA:

Overall probability: 0.727
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLY26	0.00	1.00
TYR27	1.00	1.00
GLN28	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
G26HA2	1.00
G26HA3	1.00
Y27HB2	1.00
Y27HB3	1.00
Y27HD1	1.00
Y27HD2	1.00
Y27H	1.00
Y27HA	1.00
Q28H	1.00
Q28HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLY26	HA2	1.00	0.441	0.00	0.00
GLY26	HA3	1.00	0.309	0.00	0.00
TYR27	HA	1.00	0.002	1.00	6.50
TYR27	HB2	1.00	0.004	1.00	0.30
TYR27	HB3	1.00	0.002	1.00	0.30
TYR27	HD1	1.00	0.013	1.00	0.17
TYR27	HD2	1.00	0.013	1.00	0.17
TYR27	H	1.00	0.023	1.00	0.13
TYR27	HE1	0.75	0.023	1.00	0.14
GLN28	HA	1.00	0.048	0.00	0.00
GLN28	H	1.00	0.006	1.00	0.81

3.27.2 Detailed Probabilities of TYR27CB:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR27	0.86	1.00
GLN28	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y27HA	1.00
Y27HB2	1.00
Y27HD1	1.00
Y27HD2	1.00
Y27HE2	1.00
Y27H	1.00
Y27HB3	1.00
Q28H	1.00

NOESY contacts detailed probability

3.27 TYR(27)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR27	HA	1.00	0.001	1.00	0.19
TYR27	HB2	1.00	0.004	1.00	0.63
TYR27	HB3	1.00	0.007	1.00	1.01
TYR27	HD1	1.00	0.009	1.00	0.37
TYR27	HD2	1.00	0.009	1.00	0.37
TYR27	HE2	1.00	0.210	0.00	0.00
TYR27	H	1.00	0.016	1.00	0.13
GLN28	H	1.00	0.004	1.00	0.16

3.27.3 Detailed Probabilities of TYR27CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR27	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y27HA	1.00
Y27HB2	1.00
Y27HB3	1.00
Y27HD2	1.00
Y27HE1	1.00
Y27HE2	1.00
Y27H	1.00
Y27HD1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR27	HA	1.00	0.005	1.00	0.19
TYR27	HB2	1.00	0.010	1.00	0.77
TYR27	HB3	1.00	0.002	1.00	0.95
TYR27	HD1	1.00	0.007	1.00	7.88
TYR27	HD2	1.00	0.007	1.00	7.88
TYR27	HE1	1.00	0.007	1.00	2.85
TYR27	HE2	1.00	0.007	1.00	2.85
TYR27	H	1.00	0.015	1.00	0.49

3.27.4 Detailed Probabilities of TYR27CD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR27	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y27HA	1.00
Y27HB2	1.00
Y27HB3	1.00
Y27HD1	1.00
Y27HE1	1.00
Y27HE2	1.00
Y27H	0.98
Y27HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR27	HA	1.00	0.005	1.00	0.19
TYR27	HB2	1.00	0.010	1.00	0.77
TYR27	HB3	1.00	0.002	1.00	0.95
TYR27	HD1	1.00	0.007	1.00	7.88
TYR27	HD2	1.00	0.007	1.00	7.88
TYR27	HE1	1.00	0.007	1.00	2.85
TYR27	HE2	1.00	0.007	1.00	2.85
TYR27	H	0.98	0.015	1.00	0.49

3.27.5 Detailed Probabilities of TYR27CE1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR27	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y27HD1	1.00
Y27HD2	1.00
Y27HE2	1.00
Y27HE1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR27	HD1	1.00	0.006	1.00	2.58
TYR27	HD2	1.00	0.006	1.00	2.58
TYR27	HE1	1.00	0.002	1.00	8.29
TYR27	HE2	1.00	0.002	1.00	8.29
TYR27	HB2	0.89	0.015	1.00	0.28
TYR27	HB3	0.88	0.001	1.00	0.35

3.27.6 Detailed Probabilities of TYR27CE2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR27	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y27HB2	1.00
Y27HB3	1.00
Y27HD1	1.00
Y27HD2	1.00
Y27HE1	1.00
Y27HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR27	HB2	1.00	0.015	1.00	0.28
TYR27	HB3	1.00	0.001	1.00	0.35
TYR27	HD1	1.00	0.006	1.00	2.58
TYR27	HD2	1.00	0.006	1.00	2.58
TYR27	HE1	1.00	0.002	1.00	8.29
TYR27	HE2	1.00	0.002	1.00	8.29

3.27.7 Detailed Probabilities of TYR27N:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLY26	0.33	1.00
TYR27	0.50	1.00
GLN28	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
G26HA2	1.00
G26HA3	1.00
G26H	1.00
Y27HA	1.00
Y27HB2	1.00
Y27HB3	1.00
Y27HD1	1.00
Y27HD2	0.98
Y27H	1.00
Q28H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLY26	HA2	1.00	0.022	1.00	-98922.00
GLY26	HA3	1.00	0.289	0.00	0.00
GLY26	H	1.00	0.317	0.00	0.00
TYR27	HA	1.00	0.596	0.00	0.00
TYR27	HB2	1.00	0.003	1.00	-143664.00
TYR27	HB3	1.00	0.294	0.00	0.00
TYR27	HD1	1.00	0.008	1.00	-182314.00
TYR27	HD2	0.98	0.008	1.00	-182314.00
TYR27	H	1.00	0.492	0.00	0.00
GLN28	H	1.00	0.001	1.00	-77799.00

3.27.8 Detailed Probabilities of TYR27HA:

Overall probability: 0.700

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLY26	0.50	1.00
TYR27	0.83	1.00
GLN28	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
G26HA2	1.00
G26HA3	1.00
Y27HB2	1.00
Y27HB3	1.00
Y27HD1	1.00
Y27HD2	1.00
Y27H	1.00
Y27HA	1.00
Q28H	1.00
Q28HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLY26	HA2	1.00	0.018	1.00	0.05
GLY26	HA3	1.00	0.148	0.00	0.00
TYR27	HA	1.00	0.002	1.00	6.50
TYR27	HB2	1.00	0.008	1.00	0.17
TYR27	HB3	1.00	0.001	1.00	0.19
TYR27	HD1	1.00	0.005	1.00	0.19
TYR27	HD2	1.00	0.005	1.00	0.19
TYR27	H	1.00	0.596	0.00	0.00
GLN28	HA	1.00	0.069	0.00	0.00
GLN28	H	1.00	0.004	1.00	-1201791.00

3.27.9 Detailed Probabilities of TYR27HB2:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR27	0.88	1.00
GLN28	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
Y27HA	1.00
Y27HB3	1.00
Y27HD1	1.00
Y27HD2	1.00
Y27HE2	1.00
Y27H	1.00
Y27HB2	1.00
Q28H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR27	HA	1.00	0.004	1.00	0.30
TYR27	HB2	1.00	0.156	0.00	0.00
TYR27	HB3	1.00	0.004	1.00	0.63
TYR27	HD1	1.00	0.010	1.00	0.77
TYR27	HD2	1.00	0.010	1.00	0.77
TYR27	HE2	1.00	0.015	1.00	0.28
TYR27	H	1.00	0.003	1.00	-143664.00
TYR27	HE1	0.89	0.015	1.00	0.28
GLN28	H	1.00	0.081	0.00	0.00
GLN28	HA	0.57	0.004	1.00	0.77

3.27.10 Detailed Probabilities of TYR27HB3:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR27	0.88	1.00
GLN28	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y27HA	1.00
Y27HB2	1.00
Y27HD1	1.00
Y27HD2	1.00
Y27HE2	1.00
Y27H	1.00
Y27HB3	1.00
Q28H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR27	HA	1.00	0.002	1.00	0.30
TYR27	HB2	1.00	0.002	1.00	0.60
TYR27	HB3	1.00	0.007	1.00	1.01
TYR27	HD1	1.00	0.002	1.00	0.95
TYR27	HD2	1.00	0.002	1.00	0.95
TYR27	HE2	1.00	0.001	1.00	0.35
TYR27	H	1.00	0.294	0.00	0.00
TYR27	HE1	0.88	0.001	1.00	0.35
GLN28	H	1.00	0.005	1.00	-285476.00
GLN28	HA	0.81	0.019	1.00	0.15

3.27.11 Detailed Probabilities of TYR27HD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR27	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y27HA	1.00
Y27HB2	1.00
Y27HB3	1.00
Y27HD2	1.00
Y27HE1	1.00
Y27HE2	1.00
Y27H	1.00
Y27HD1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR27	HA	1.00	0.013	1.00	0.17
TYR27	HB2	1.00	0.009	1.00	0.25
TYR27	HB3	1.00	0.009	1.00	0.37
TYR27	HD1	1.00	0.007	1.00	7.88
TYR27	HD2	1.00	0.007	1.00	7.88
TYR27	HE1	1.00	0.006	1.00	2.58
TYR27	HE2	1.00	0.006	1.00	2.58
TYR27	H	1.00	0.008	1.00	-182314.00

3.27.12 Detailed Probabilities of TYR27HD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR27	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y27HA	1.00
Y27HB2	1.00
Y27HB3	1.00
Y27HD1	1.00
Y27HE1	1.00
Y27HE2	1.00
Y27H	0.98
Y27HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR27	HA	1.00	0.013	1.00	0.17
TYR27	HB2	1.00	0.009	1.00	0.25
TYR27	HB3	1.00	0.009	1.00	0.37
TYR27	HD1	1.00	0.007	1.00	7.88
TYR27	HD2	1.00	0.007	1.00	7.88
TYR27	HE1	1.00	0.006	1.00	2.58
TYR27	HE2	1.00	0.006	1.00	2.58
TYR27	H	0.98	0.008	1.00	-182314.00

3.27.13 Detailed Probabilities of TYR27HE1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR27	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y27HD1	1.00
Y27HD2	1.00
Y27HE2	1.00
Y27HE1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR27	HD1	1.00	0.007	1.00	2.85
TYR27	HD2	1.00	0.007	1.00	2.85
TYR27	HE1	1.00	0.002	1.00	8.29
TYR27	HE2	1.00	0.002	1.00	8.29
TYR27	HA	0.75	0.023	1.00	0.14
TYR27	HB2	0.89	0.011	1.00	0.07

3.27.14 Detailed Probabilities of TYR27HE2:

Overall probability: 0.834

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR27	0.83	1.00

Expected NOESY Contacts

Proton	Expected probability
Y27HB2	1.00
Y27HB3	1.00
Y27HD1	1.00
Y27HD2	1.00
Y27HE1	1.00
Y27HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR27	HB2	1.00	0.011	1.00	0.07
TYR27	HB3	1.00	0.210	0.00	0.00
TYR27	HD1	1.00	0.007	1.00	2.85
TYR27	HD2	1.00	0.007	1.00	2.85
TYR27	HE1	1.00	0.002	1.00	8.29
TYR27	HE2	1.00	0.002	1.00	8.29

3.27.15 Detailed Probabilities of TYR27H:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLY26	0.00	1.00
TYR27	0.83	1.00
GLN28	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
G26HA2	1.00
G26HA3	1.00
G26H	1.00
Y27HA	1.00
Y27HB2	1.00
Y27HB3	1.00
Y27HD1	1.00
Y27HD2	0.98
Y27H	1.00
Q28H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLY26	HA2	1.00	0.082	0.00	0.00
GLY26	HA3	1.00	0.058	0.00	0.00
GLY26	H	1.00	0.183	0.00	0.00
TYR27	HA	1.00	0.023	1.00	0.13
TYR27	HB2	1.00	0.002	1.00	0.12
TYR27	HB3	1.00	0.016	1.00	0.13
TYR27	HD1	1.00	0.015	1.00	0.49
TYR27	HD2	0.98	0.015	1.00	0.49
TYR27	H	1.00	0.492	0.00	0.00
GLN28	H	1.00	0.273	0.00	0.00

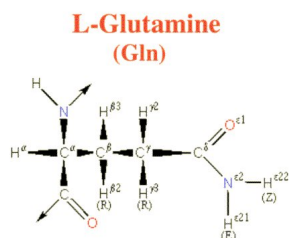
3.28 GLN(28)

Figure 27: Image from the BMRB

Residue probability: 0.729

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.625	176.405	1.998	0.000	0.000
CA 3.28.1	54.380	56.667	2.318	0.883	1.000
CB 3.28.2	30.455	29.436	2.799	0.778	1.000
CG 3.28.3	33.720	33.781	1.871	0.778	1.000
N 3.28.4	120.362	119.799	3.762	0.600	1.000
NE2 3.28.5	113.892	111.924	2.434	0.833	1.000
HA 3.28.6	4.499	4.265	0.455	0.600	1.000
HB2 3.28.7	2.062	2.047	0.290	0.778	1.000
HB3 3.28.8	1.783	2.012	0.313	0.540	1.000
HG2 3.28.9	2.239	2.308	0.289	0.833	1.000
HG3 3.28.10	2.202	2.284	0.313	0.700	1.000
H 3.28.11	8.338	8.232	0.711	0.769	1.000
HE21 3.28.12	7.522	7.217	0.496	0.717	1.000
HE22 3.28.13	7.013	7.041	0.463	0.667	1.000

3.28.1 Detailed Probabilities of GLN28CA:

Overall probability: 0.883

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR27	0.67	1.00
GLN28	0.93	1.00
VAL29	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y27HA	1.00
Q28HB2	1.00
Q28HB3	1.00
Q28HG2	1.00
Q28HG3	1.00
Q28H	1.00
Q28HA	1.00
V29HA	1.00
V29H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR27	HA	1.00	0.069	0.00	0.00
TYR27	HB2	0.57	0.004	1.00	0.77
TYR27	HB3	0.81	0.019	1.00	0.15
GLN28	HA	1.00	0.003	1.00	10.31
GLN28	HB2	1.00	0.000	1.00	0.61
GLN28	HB3	1.00	0.003	1.00	0.45
GLN28	HG2	1.00	0.003	1.00	0.51
GLN28	HG3	1.00	0.034	0.60	0.00
GLN28	H	1.00	0.009	1.00	0.35
VAL29	HA	1.00	0.000	1.00	0.21
VAL29	H	1.00	0.002	1.00	1.60
VAL29	HG21	0.53	0.005	1.00	0.47

3.28.2 Detailed Probabilities of GLN28CB:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN28	0.88	1.00
VAL29	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q28HA	1.00
Q28HB2	1.00
Q28HG2	1.00
Q28HG3	1.00
Q28H	1.00
Q28HE21	1.00
Q28HE22	1.00
Q28HB3	1.00
V29H	1.00

NOESY contacts detailed probability

3.28 GLN(28)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN28	HA	1.00	0.002	1.00	0.38
GLN28	HB2	1.00	0.001	1.00	1.49
GLN28	HB3	1.00	0.004	1.00	2.36
GLN28	HG2	1.00	0.010	1.00	0.72
GLN28	HG3	1.00	0.027	1.00	0.72
GLN28	H	1.00	0.006	1.00	0.30
GLN28	HE21	1.00	0.007	1.00	0.06
GLN28	HE22	1.00	0.502	0.00	0.00
VAL29	H	1.00	0.432	0.00	0.00

3.28.3 Detailed Probabilities of GLN28CG:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN28	0.75	1.00
VAL29	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q28HA	1.00
Q28HB2	1.00
Q28HB3	1.00
Q28HG3	1.00
Q28H	1.00
Q28HE21	1.00
Q28HE22	1.00
Q28HG2	1.00
V29H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN28	HA	1.00	0.003	1.00	0.31
GLN28	HB2	1.00	0.183	0.00	0.00
GLN28	HB3	1.00	0.010	1.00	0.69
GLN28	HG2	1.00	0.006	1.00	7.01
GLN28	HG3	1.00	0.043	0.00	0.00
GLN28	H	1.00	0.006	1.00	0.27
GLN28	HE21	1.00	0.006	1.00	0.39
GLN28	HE22	1.00	0.001	1.00	0.10
VAL29	H	0.98	0.005	1.00	0.09

3.28.4 Detailed Probabilities of GLN28N:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR27	0.67	1.00
GLN28	0.57	1.00
VAL29	0.40	1.00

Expected NOESY Contacts

Proton	Expected probability
Y27HB3	1.00
Y27H	1.00
Y27HA	1.00
Y27HB2	1.00
Q28HA	1.00
Q28HB2	1.00
Q28HB3	1.00
Q28HG2	1.00
Q28HG3	1.00
Q28H	1.00
V29H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR27	HA	1.00	0.004	1.00	-1201791.00
TYR27	HB2	1.00	0.081	0.00	0.00
TYR27	HB3	1.00	0.005	1.00	-285476.00
TYR27	H	1.00	0.273	0.00	0.00
TYR27	HD1	0.78	0.007	1.00	-116364.00
TYR27	HD2	0.71	0.007	1.00	-116364.00
GLN28	HA	1.00	0.062	0.00	0.00
GLN28	HB2	1.00	0.003	1.00	-386719.00
GLN28	HB3	1.00	0.036	0.40	0.00
GLN28	HG2	1.00	0.014	1.00	-433907.00
GLN28	HG3	1.00	0.023	1.00	-433907.00
GLN28	H	1.00	0.402	0.00	0.00
VAL29	H	1.00	0.036	0.40	0.00

3.28.5 Detailed Probabilities of GLN28NE2:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN28	0.83	1.00

Expected NOESY Contacts

Proton	Expected probability
Q28HB2	1.00
Q28HB3	1.00
Q28HG2	1.00
Q28HG3	1.00
Q28HE22	1.00
Q28HE21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN28	HB2	1.00	0.004	1.00	-169636.00
GLN28	HB3	1.00	0.283	0.00	0.00
GLN28	HG2	1.00	0.013	1.00	-515742.00
GLN28	HG3	1.00	0.024	1.00	-515742.00
GLN28	HE21	1.00	0.008	1.00	-7095362.00
GLN28	HE22	1.00	0.004	1.00	-4704666.00

3.28.6 Detailed Probabilities of GLN28HA:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR27	0.00	1.00
GLN28	0.67	1.00
VAL29	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
Y27HA	1.00
Q28HB2	1.00
Q28HB3	1.00
Q28HG2	1.00
Q28HG3	1.00
Q28H	1.00
Q28HA	1.00
V29HA	1.00
V29H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR27	HA	1.00	0.048	0.00	0.00
GLN28	HA	1.00	0.003	1.00	10.31
GLN28	HB2	1.00	0.010	1.00	0.90
GLN28	HB3	1.00	0.002	1.00	0.38
GLN28	HG2	1.00	0.003	1.00	0.31
GLN28	HG3	1.00	0.552	0.00	0.00
GLN28	H	1.00	0.062	0.00	0.00
VAL29	HA	1.00	0.043	0.00	0.00
VAL29	H	1.00	0.002	1.00	-2199222.00
VAL29	HG21	0.53	0.013	1.00	1.03

3.28.7 Detailed Probabilities of GLN28HB2:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN28	0.75	1.00
VAL29	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q28HA	1.00
Q28HB3	1.00
Q28HG2	1.00
Q28HG3	1.00
Q28H	1.00
Q28HE21	1.00
Q28HE22	1.00
Q28HB2	1.00
V29H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN28	HA	1.00	0.000	1.00	0.61
GLN28	HB2	1.00	0.437	0.00	0.00
GLN28	HB3	1.00	0.001	1.00	1.49
GLN28	HG2	1.00	0.183	0.00	0.00
GLN28	HG3	1.00	0.024	1.00	4.04
GLN28	H	1.00	0.003	1.00	-386719.00
GLN28	HE21	1.00	0.004	1.00	-169636.00
GLN28	HE22	1.00	0.016	1.00	-83938.00
VAL29	H	1.00	0.004	1.00	-340315.00

3.28.8 Detailed Probabilities of GLN28HB3:

Overall probability: 0.540

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN28	0.43	1.00
VAL29	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q28HA	1.00
Q28HB2	1.00
Q28HG2	1.00
Q28HG3	1.00
Q28H	1.00
Q28HE21	1.00
Q28HE22	1.00
Q28HB3	1.00
V29H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN28	HA	1.00	0.003	1.00	0.45
GLN28	HB2	1.00	0.219	0.00	0.00
GLN28	HB3	1.00	0.004	1.00	2.36
GLN28	HG2	1.00	0.010	1.00	0.69
GLN28	HG3	1.00	0.104	0.00	0.00
GLN28	H	1.00	0.036	0.40	0.00
GLN28	HE21	1.00	0.283	0.00	0.00
GLN28	HE22	1.00	0.195	0.00	0.00
VAL29	H	1.00	0.026	1.00	-110150.00
VAL29	HA	0.85	0.021	1.00	0.32

3.28.9 Detailed Probabilities of GLN28HG2:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN28	0.81	1.00
VAL29	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q28HA	1.00
Q28HB2	1.00
Q28HB3	1.00
Q28HG3	1.00
Q28H	1.00
Q28HE21	1.00
Q28HE22	1.00
Q28HG2	1.00
V29H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN28	HA	1.00	0.003	1.00	0.51
GLN28	HB2	1.00	0.260	0.00	0.00
GLN28	HB3	1.00	0.010	1.00	0.72
GLN28	HG2	1.00	0.006	1.00	7.01
GLN28	HG3	1.00	0.035	0.50	0.00
GLN28	H	1.00	0.014	1.00	-433907.00
GLN28	HE21	1.00	0.013	1.00	-515742.00
GLN28	HE22	1.00	0.005	1.00	-239856.00
VAL29	H	0.98	0.006	1.00	-212886.00

3.28.10 Detailed Probabilities of GLN28HG3:

Overall probability: 0.700

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN28	0.68	1.00
VAL29	0.90	1.00

Expected NOESY Contacts

Proton	Expected probability
Q28HA	1.00
Q28HB2	1.00
Q28HB3	1.00
Q28HG2	1.00
Q28H	1.00
Q28HE21	1.00
Q28HE22	1.00
Q28HG3	1.00
V29H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN28	HA	1.00	0.034	0.60	0.00
GLN28	HB2	1.00	0.297	0.00	0.00
GLN28	HB3	1.00	0.027	1.00	0.72
GLN28	HG2	1.00	0.043	0.00	0.00
GLN28	HG3	1.00	0.002	1.00	7.09
GLN28	H	1.00	0.023	1.00	-433907.00
GLN28	HE21	1.00	0.024	1.00	-515742.00
GLN28	HE22	1.00	0.032	0.80	0.00
VAL29	H	0.96	0.031	0.90	0.00

3.28.11 Detailed Probabilities of GLN28H:

Overall probability: 0.769

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR27	0.83	1.00
GLN28	0.67	1.00
VAL29	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y27HB3	1.00
Y27H	1.00
Y27HA	1.00
Y27HB2	1.00
Q28HA	1.00
Q28HB2	1.00
Q28HB3	1.00
Q28HG2	1.00
Q28HG3	1.00
Q28H	1.00
V29H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR27	HA	1.00	0.006	1.00	0.81
TYR27	HB2	1.00	0.491	0.00	0.00
TYR27	HB3	1.00	0.004	1.00	0.16
TYR27	H	1.00	0.001	1.00	-77799.00
TYR27	HD1	0.78	0.002	1.00	0.14
TYR27	HD2	0.71	0.002	1.00	0.14
GLN28	HA	1.00	0.009	1.00	0.35
GLN28	HB2	1.00	0.004	1.00	0.41
GLN28	HB3	1.00	0.006	1.00	0.30
GLN28	HG2	1.00	0.006	1.00	0.27
GLN28	HG3	1.00	0.051	0.00	0.00
GLN28	H	1.00	0.402	0.00	0.00
VAL29	H	1.00	0.003	1.00	-112099.00

3.28.12 Detailed Probabilities of GLN28HE21:

Overall probability: 0.717

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN28	0.72	1.00

Expected NOESY Contacts

Proton	Expected probability
Q28HB2	1.00
Q28HB3	1.00
Q28HG2	1.00
Q28HG3	1.00
Q28HE22	1.00
Q28HE21	1.00

NOESY contacts detailed probability

3.28 GLN(28)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN28	HB2	1.00	0.037	0.30	0.00
GLN28	HB3	1.00	0.007	1.00	0.06
GLN28	HG2	1.00	0.006	1.00	0.39
GLN28	HG3	1.00	0.298	0.00	0.00
GLN28	HE21	1.00	0.008	1.00	-7095362.00
GLN28	HE22	1.00	0.009	1.00	-4198795.00

3.28.13 Detailed Probabilities of GLN28HE22:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN28	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
Q28HB2	1.00
Q28HB3	1.00
Q28HG2	1.00
Q28HG3	1.00
Q28HE21	1.00
Q28HE22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN28	HB2	1.00	0.003	1.00	0.08
GLN28	HB3	1.00	0.502	0.00	0.00
GLN28	HG2	1.00	0.001	1.00	0.10
GLN28	HG3	1.00	0.001	1.00	0.10
GLN28	HE21	1.00	0.004	1.00	-4704666.00
GLN28	HE22	1.00	0.122	0.00	0.00

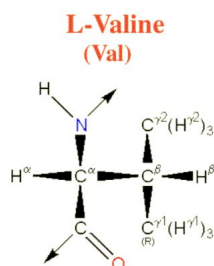
3.29 VAL(29)

Figure 28: Image from the BMRB

Residue probability: 0.828

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	175.820	175.682	2.367	0.000	0.000
CA 3.29.1	61.488	62.613	4.828	0.789	1.000
CB 3.29.2	32.473	32.918	4.591	0.833	1.000
CG1 3.29.3	21.461	21.563	2.746	0.857	1.000
CG2 3.29.4	21.871	21.368	2.801	0.800	1.000
N 3.29.5	123.482	121.057	5.832	0.908	1.000
HA 3.29.6	5.043	4.178	0.599	0.889	1.000
HB 3.29.7	1.953	1.980	0.322	0.683	1.000
HG1 3.29.8	0.800	0.816	0.264	0.857	1.000
HG2 3.29.9	0.896	0.803	0.504	0.800	1.000
H 3.29.10	8.776	8.311	0.669	0.867	1.000

3.29.1 Detailed Probabilities of VAL29CA:

Overall probability: 0.789

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN28	0.50	1.00
VAL29	0.82	1.00
ARG30	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q28HA	1.00
V29HG11	1.00
V29HG21	1.00
V29H	1.00
V29HB	1.00
V29HA	1.00
R30HA	1.00
R30H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN28	HA	1.00	0.043	0.00	0.00
GLN28	HB3	0.85	0.021	1.00	0.32
VAL29	HA	1.00	0.004	1.00	2.38
VAL29	HB	1.00	0.039	0.10	0.00
VAL29	HG11	1.00	0.004	1.00	0.83
VAL29	HG21	1.00	0.004	1.00	0.49
VAL29	H	1.00	0.018	1.00	0.20
ARG30	HA	1.00	0.011	1.00	0.10
ARG30	H	1.00	0.005	1.00	1.04

3.29.2 Detailed Probabilities of VAL29CB:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL29	0.80	1.00
ARG30	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V29HA	1.00
V29HG11	1.00
V29HG21	1.00
V29H	1.00
V29HB	1.00
R30H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL29	HA	1.00	0.011	1.00	0.06
VAL29	HB	1.00	0.270	0.00	0.00
VAL29	HG11	1.00	0.006	1.00	1.86
VAL29	HG21	1.00	0.002	1.00	1.68
VAL29	H	1.00	0.005	1.00	1.02
ARG30	H	1.00	0.004	1.00	0.11

3.29.3 Detailed Probabilities of VAL29CG1:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL29	0.80	1.00
ARG30	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V29HA	1.00
V29HG12	1.00
V29HG21	1.00
V29H	1.00
V29HB	1.00
R30H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL29	HA	1.00	0.003	1.00	1.07
VAL29	HB	1.00	0.002	1.00	2.07
VAL29	HG11	1.00	0.012	1.00	88.89
VAL29	HG21	1.00	0.084	0.00	0.00
VAL29	H	1.00	0.003	1.00	0.42
ARG30	H	0.98	0.001	1.00	0.61
ARG30	HA	0.56	0.001	1.00	0.23

3.29.4 Detailed Probabilities of VAL29CG2:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL29	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
V29HA	1.00
V29HG11	1.00
V29HG22	1.00
V29H	1.00
V29HB	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL29	HA	1.00	0.002	1.00	0.76
VAL29	HB	1.00	0.001	1.00	3.29
VAL29	HG11	1.00	0.309	0.00	0.00
VAL29	HG21	1.00	0.017	1.00	78.79
VAL29	H	1.00	0.001	1.00	0.70

3.29.5 Detailed Probabilities of VAL29N:

Overall probability: 0.908

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN28	0.98	1.00
VAL29	1.00	1.00
ARG30	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q28HG3	0.96
Q28H	1.00
Q28HG2	0.98
Q28HA	1.00
Q28HB2	1.00
Q28HB3	1.00
V29HA	1.00
V29HG11	1.00
V29HG21	1.00
V29HB	1.00
V29H	1.00
R30H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN28	HA	1.00	0.002	1.00	-2199222.00
GLN28	HB2	1.00	0.004	1.00	-340315.00
GLN28	HB3	1.00	0.026	1.00	-110150.00
GLN28	HG2	0.98	0.006	1.00	-212886.00
GLN28	HG3	0.96	0.031	0.90	0.00
GLN28	H	1.00	0.003	1.00	-112099.00
VAL29	HA	1.00	0.005	1.00	-372461.00
VAL29	HB	1.00	0.001	1.00	-1152839.00
VAL29	HG11	1.00	0.007	1.00	-387603.00
VAL29	HG21	1.00	0.001	1.00	-1043999.00
VAL29	H	1.00	0.000	1.00	-6232856.00
ARG30	H	1.00	0.043	0.00	0.00

3.29.6 Detailed Probabilities of VAL29HA:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN28	1.00	1.00
VAL29	1.00	1.00
ARG30	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
Q28HA	1.00
V29HG11	1.00
V29HG21	1.00
V29H	1.00
V29HB	1.00
V29HA	1.00
R30HA	1.00
R30H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN28	HA	1.00	0.000	1.00	0.21
VAL29	HA	1.00	0.004	1.00	2.38
VAL29	HB	1.00	0.011	1.00	0.06
VAL29	HG11	1.00	0.003	1.00	1.07
VAL29	HG21	1.00	0.002	1.00	0.76
VAL29	H	1.00	0.005	1.00	-372461.00
ARG30	HA	1.00	0.085	0.00	0.00
ARG30	H	1.00	0.005	1.00	-2123519.00
ARG30	HB2	0.54	0.005	1.00	0.08

3.29.7 Detailed Probabilities of VAL29HB:

Overall probability: 0.683

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL29	0.62	1.00
ARG30	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V29HA	1.00
V29HG11	1.00
V29HG21	1.00
V29H	1.00
V29HB	1.00
R30H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL29	HA	1.00	0.039	0.10	0.00
VAL29	HB	1.00	0.270	0.00	0.00
VAL29	HG11	1.00	0.002	1.00	2.07
VAL29	HG21	1.00	0.001	1.00	3.29
VAL29	H	1.00	0.001	1.00	-1152839.00
ARG30	H	1.00	0.005	1.00	-155074.00

3.29.8 Detailed Probabilities of VAL29HG11:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL29	0.80	1.00
ARG30	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V29HA	1.00
V29HG12	1.00
V29HG21	1.00
V29H	1.00
V29HB	1.00
R30H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL29	HA	1.00	0.004	1.00	0.83
VAL29	HB	1.00	0.006	1.00	1.86
VAL29	HG11	1.00	0.012	1.00	88.89
VAL29	HG21	1.00	0.309	0.00	0.00
VAL29	H	1.00	0.007	1.00	-387603.00
ARG30	H	0.98	0.008	1.00	-796220.00
ARG30	HA	0.56	0.015	1.00	0.56

3.29.9 Detailed Probabilities of VAL29HG21:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL29	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
V29HA	1.00
V29HG11	1.00
V29HG22	1.00
V29H	1.00
V29HB	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL29	HA	1.00	0.004	1.00	0.49
VAL29	HB	1.00	0.002	1.00	1.68
VAL29	HG11	1.00	0.084	0.00	0.00
VAL29	HG21	1.00	0.017	1.00	78.79
VAL29	H	1.00	0.001	1.00	-1043999.00

3.29.10 Detailed Probabilities of VAL29H:

Overall probability: 0.867

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN28	0.73	1.00
VAL29	1.00	1.00
ARG30	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q28HG3	0.96
Q28H	1.00
Q28HG2	0.98
Q28HA	1.00
Q28HB2	1.00
Q28HB3	1.00
V29HA	1.00
V29HG11	1.00
V29HG21	1.00
V29HB	1.00
V29H	1.00
R30H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN28	HA	1.00	0.002	1.00	1.60
GLN28	HB2	1.00	0.002	1.00	0.15
GLN28	HB3	1.00	0.432	0.00	0.00
GLN28	HG2	0.98	0.005	1.00	0.09
GLN28	HG3	0.96	0.013	1.00	0.06
GLN28	H	1.00	0.036	0.40	0.00
VAL29	HA	1.00	0.018	1.00	0.20
VAL29	HB	1.00	0.005	1.00	1.02
VAL29	HG11	1.00	0.003	1.00	0.42
VAL29	HG21	1.00	0.001	1.00	0.70
VAL29	H	1.00	0.000	1.00	-6232856.00
ARG30	H	1.00	0.001	1.00	-124543.00

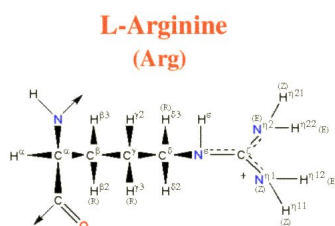


Figure 29: Image from the BMRB

Residue probability: 0.622
Residue probability confidence: 0.866

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	173.332	176.453	2.303	0.000	0.000
CA 3.30.1	53.788	56.803	3.326	0.388	1.000
CB 3.30.2	32.391	30.892	2.424	0.778	0.900
CG 3.30.3	26.702	27.247	1.538	0.449	0.818
CD 3.30.4	42.856	43.189	1.415	0.850	0.700
N 3.30.5	127.787	120.701	3.779	0.923	1.000
NE	NA	—	—	0.000	0.000
NH1	NA	—	—	0.000	0.000
NH2	NA	—	—	0.000	0.000
HA 3.30.6	4.740	4.301	0.495	0.860	1.000
HB2 3.30.7	1.654	1.793	0.292	0.400	0.900
HB3 3.30.8	1.514	1.757	0.307	0.500	0.900
HG2 3.30.9	1.497	1.559	0.294	0.444	0.818
HG3 3.30.10	1.452	1.535	0.310	0.071	0.818
HD2 3.30.11	3.333	3.105	0.301	0.914	0.700
HD3 3.30.12	2.933	3.081	0.306	0.575	0.700
H 3.30.13	9.135	8.248	0.623	0.929	1.000
HE	NA	—	—	0.000	0.000
HH1	NA	—	—	0.000	0.000
HH2	NA	—	—	0.000	0.000

3.30.1 Detailed Probabilities of ARG30CA:

Overall probability: 0.388
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL29	0.64	1.00
ARG30	0.39	1.00
ASP31	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V29HA	1.00
R30HB2	1.00
R30HB3	1.00
R30HG2	1.00
R30HG3	1.00
R30HD2	0.98
R30HD3	0.97
R30H	1.00
R30HA	1.00
D31H	1.00
D31HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL29	HA	1.00	0.085	0.00	0.00
VAL29	HG11	0.57	0.015	1.00	0.56
VAL29	H	0.92	0.031	0.92	0.00
ARG30	HA	1.00	0.004	1.00	4.38
ARG30	HB2	1.00	0.034	0.60	0.00
ARG30	HB3	1.00	0.052	0.00	0.00
ARG30	HG2	1.00	0.069	0.00	0.00
ARG30	HG3	1.00	0.039	0.10	0.00
ARG30	HD2	0.98	0.036	0.40	0.00
ARG30	HD3	0.97	0.095	0.03	0.00
ARG30	H	1.00	0.013	1.00	0.48
ASP31	HA	1.00	0.082	0.00	0.00
ASP31	H	1.00	0.043	0.00	0.00

3.30.2 Detailed Probabilities of ARG30CB:

Overall probability: 0.778

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG30	0.75	0.89
ASP31	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R30HA	1.00
R30HB3	1.00
R30HG2	1.00
R30HG3	1.00
R30HD2	1.00
R30HD3	1.00
R30H	1.00
R30HE	1.00
R30HB2	1.00
D31H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG30	HA	1.00	0.010	1.00	0.21
ARG30	HB2	1.00	0.137	0.00	0.00
ARG30	HB3	1.00	0.003	1.00	0.68
ARG30	HG2	1.00	0.020	1.00	0.68
ARG30	HG3	1.00	0.065	0.00	0.00
ARG30	HD2	1.00	0.005	1.00	0.09
ARG30	HD3	1.00	0.006	1.00	0.14
ARG30	H	1.00	0.006	1.00	0.08
ASP31	H	1.00	0.008	1.00	0.06

3.30.3 Detailed Probabilities of ARG30CG:

Overall probability: 0.449

Overall confidence: 0.818

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG30	0.50	0.80
ASP31	0.04	1.00

Expected NOESY Contacts

Proton	Expected probability
R30HA	1.00
R30HB2	1.00
R30HB3	1.00
R30HG2	1.00
R30HD2	1.00
R30HD3	1.00
R30H	1.00
R30HE	1.00
R30HH11	1.00
R30HG3	1.00
D31H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG30	HA	1.00	0.007	1.00	0.22
ARG30	HB2	1.00	0.242	0.00	0.00
ARG30	HB3	1.00	0.256	0.00	0.00
ARG30	HG2	1.00	0.239	0.00	0.00
ARG30	HG3	1.00	0.194	0.00	0.00
ARG30	HD2	1.00	0.005	1.00	0.18
ARG30	HD3	1.00	0.008	1.00	0.19
ARG30	H	1.00	0.006	1.00	0.11
ASP31	H	0.96	0.556	0.04	0.00

3.30.4 Detailed Probabilities of ARG30CD:

Overall probability: 0.850

Overall confidence: 0.700

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG30	0.85	0.70

Expected NOESY Contacts

Proton	Expected probability
R30HA	0.98
R30HB2	1.00
R30HB3	1.00
R30HG2	1.00
R30HG3	1.00
R30HD3	1.00
R30HE	1.00
R30HH11	1.00
R30HH21	1.00
R30HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG30	HA	0.98	0.037	0.30	0.00
ARG30	HB2	1.00	0.009	1.00	0.26
ARG30	HB3	1.00	0.027	1.00	0.48
ARG30	HG2	1.00	0.010	1.00	0.48
ARG30	HG3	1.00	0.035	0.50	0.00
ARG30	HD2	1.00	0.006	1.00	2.10
ARG30	HD3	1.00	0.006	1.00	1.44
ARG30	H	0.87	0.002	1.00	0.06

3.30.5 Detailed Probabilities of ARG30N:

Overall probability: 0.923

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL29	1.00	1.00
ARG30	0.83	1.00
ASP31	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V29HG11	0.98
V29H	1.00
V29HB	1.00
V29HA	1.00
R30HA	1.00
R30HB2	1.00
R30HB3	1.00
R30HG2	1.00
R30HG3	1.00
R30H	1.00
D31H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL29	HA	1.00	0.005	1.00	-2123519.00
VAL29	HB	1.00	0.005	1.00	-155074.00
VAL29	HG11	0.98	0.008	1.00	-796220.00
VAL29	H	1.00	0.001	1.00	-124543.00
VAL29	HG21	0.94	0.002	1.00	-337086.00
ARG30	HA	1.00	0.006	1.00	-296604.00
ARG30	HB2	1.00	0.001	1.00	-269763.00
ARG30	HB3	1.00	0.016	1.00	-485219.00
ARG30	HG2	1.00	0.001	1.00	-485219.00
ARG30	HG3	1.00	0.046	0.00	0.00
ARG30	H	1.00	0.006	1.00	-4695212.00
ASP31	H	1.00	0.001	1.00	-120160.00
ASP31	HA	0.84	0.001	1.00	-98556.00

3.30.6 Detailed Probabilities of ARG30HA:

Overall probability: 0.860

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL29	1.00	1.00
ARG30	0.79	1.00
ASP31	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V29HA	1.00
R30HB2	1.00
R30HB3	1.00
R30HG2	1.00
R30HG3	1.00
R30HD2	0.98
R30HD3	0.97
R30H	1.00
R30HA	1.00
D31H	1.00
D31HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL29	HA	1.00	0.011	1.00	0.10
VAL29	HG11	0.57	0.001	1.00	0.23
ARG30	HA	1.00	0.004	1.00	4.38
ARG30	HB2	1.00	0.010	1.00	0.21
ARG30	HB3	1.00	0.003	1.00	0.16
ARG30	HG2	1.00	0.008	1.00	0.22
ARG30	HG3	1.00	0.007	1.00	0.22
ARG30	HD2	0.98	0.037	0.30	0.00
ARG30	HD3	0.97	0.546	0.03	0.00
ARG30	H	1.00	0.006	1.00	-296604.00
ASP31	HA	1.00	0.009	1.00	0.06
ASP31	H	1.00	0.009	1.00	-2142537.00

3.30.7 Detailed Probabilities of ARG30HB2:

Overall probability: 0.400

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG30	0.33	0.89
ASP31	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R30HA	1.00
R30HB3	1.00
R30HG2	1.00
R30HG3	1.00
R30HD2	1.00
R30HD3	1.00
R30H	1.00
R30HE	1.00
R30HB2	1.00
D31H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG30	HA	1.00	0.034	0.60	0.00
ARG30	HB2	1.00	0.137	0.00	0.00
ARG30	HB3	1.00	0.229	0.00	0.00
ARG30	HG2	1.00	0.260	0.00	0.00
ARG30	HG3	1.00	0.242	0.00	0.00
ARG30	HD2	1.00	0.009	1.00	0.26
ARG30	HD3	1.00	0.995	0.00	0.00
ARG30	H	1.00	0.001	1.00	-269763.00
ASP31	H	1.00	0.005	1.00	-486197.00

3.30.8 Detailed Probabilities of ARG30HB3:

Overall probability: 0.500

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG30	0.38	0.89
ASP31	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R30HA	1.00
R30HB2	1.00
R30HG2	1.00
R30HG3	1.00
R30HD2	1.00
R30HD3	1.00
R30H	1.00
R30HE	1.00
R30HB3	1.00
D31H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG30	HA	1.00	0.052	0.00	0.00
ARG30	HB2	1.00	0.003	1.00	0.68
ARG30	HB3	1.00	0.369	0.00	0.00
ARG30	HG2	1.00	0.120	0.00	0.00
ARG30	HG3	1.00	0.256	0.00	0.00
ARG30	HD2	1.00	0.027	1.00	0.48
ARG30	HD3	1.00	0.855	0.00	0.00
ARG30	H	1.00	0.016	1.00	-485219.00
ASP31	H	1.00	0.004	1.00	-408723.00
ASP31	HA	0.75	0.002	1.00	0.05

3.30.9 Detailed Probabilities of ARG30HG2:

Overall probability: 0.444

Overall confidence: 0.818

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG30	0.38	0.80
ASP31	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R30HA	1.00
R30HB2	1.00
R30HB3	1.00
R30HG3	1.00
R30HD2	1.00
R30HD3	1.00
R30H	1.00
R30HE	1.00
R30HH11	1.00
R30HG2	1.00
D31H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG30	HA	1.00	0.069	0.00	0.00
ARG30	HB2	1.00	0.020	1.00	0.68
ARG30	HB3	1.00	0.386	0.00	0.00
ARG30	HG2	1.00	0.103	0.00	0.00
ARG30	HG3	1.00	0.239	0.00	0.00
ARG30	HD2	1.00	0.010	1.00	0.48
ARG30	HD3	1.00	0.838	0.00	0.00
ARG30	H	1.00	0.001	1.00	-485219.00
ASP31	H	0.98	0.013	1.00	-408723.00

3.30.10 Detailed Probabilities of ARG30HG3:

Overall probability: 0.071

Overall confidence: 0.818

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG30	0.08	0.80
ASP31	0.04	1.00

Expected NOESY Contacts

Proton	Expected probability
R30HA	1.00
R30HB2	1.00
R30HB3	1.00
R30HG2	1.00
R30HD2	1.00
R30HD3	1.00
R30H	1.00
R30HE	1.00
R30HH11	1.00
R30HG3	1.00
D31H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG30	HA	1.00	0.039	0.10	0.00
ARG30	HB2	1.00	0.065	0.00	0.00
ARG30	HB3	1.00	0.431	0.00	0.00
ARG30	HG2	1.00	0.058	0.00	0.00
ARG30	HG3	1.00	0.194	0.00	0.00
ARG30	HD2	1.00	0.035	0.50	0.00
ARG30	HD3	1.00	0.793	0.00	0.00
ARG30	H	1.00	0.046	0.00	0.00
ASP31	H	0.96	0.058	0.04	0.00

3.30.11 Detailed Probabilities of ARG30HD2:

Overall probability: 0.914

Overall confidence: 0.700

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG30	0.91	0.70

Expected NOESY Contacts

Proton	Expected probability
R30HA	0.98
R30HB2	1.00
R30HB3	1.00
R30HG2	1.00
R30HG3	1.00
R30HD3	1.00
R30HE	1.00
R30HH11	1.00
R30HH21	1.00
R30HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG30	HA	0.98	0.036	0.40	0.00
ARG30	HB2	1.00	0.005	1.00	0.09
ARG30	HB3	1.00	0.010	1.00	0.07
ARG30	HG2	1.00	0.001	1.00	0.18
ARG30	HG3	1.00	0.005	1.00	0.18
ARG30	HD2	1.00	0.006	1.00	2.10
ARG30	HD3	1.00	0.004	1.00	1.28

3.30.12 Detailed Probabilities of ARG30HD3:

Overall probability: 0.575

Overall confidence: 0.700

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG30	0.58	0.70

Expected NOESY Contacts

Proton	Expected probability
R30HA	0.97
R30HB2	1.00
R30HB3	1.00
R30HG2	1.00
R30HG3	1.00
R30HD2	1.00
R30HE	1.00
R30HH11	1.00
R30HH21	1.00
R30HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG30	HA	0.97	0.095	0.03	0.00
ARG30	HB2	1.00	0.006	1.00	0.14
ARG30	HB3	1.00	0.002	1.00	0.09
ARG30	HG2	1.00	0.399	0.00	0.00
ARG30	HG3	1.00	0.008	1.00	0.19
ARG30	HD2	1.00	0.006	1.00	1.44
ARG30	HD3	1.00	0.404	0.00	0.00

3.30.13 Detailed Probabilities of ARG30H:

Overall probability: 0.929

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL29	0.80	1.00
ARG30	1.00	1.00
ASP31	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V29HG11	0.98
V29H	1.00
V29HB	1.00
V29HA	1.00
R30HA	1.00
R30HB2	1.00
R30HB3	1.00
R30HG2	1.00
R30HG3	1.00
R30H	1.00
D31H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL29	HA	1.00	0.005	1.00	1.04
VAL29	HB	1.00	0.004	1.00	0.11
VAL29	HG11	0.98	0.001	1.00	0.61
VAL29	H	1.00	0.043	0.00	0.00
VAL29	HG21	0.94	0.012	1.00	0.22
ARG30	HA	1.00	0.013	1.00	0.48
ARG30	HB2	1.00	0.006	1.00	0.08
ARG30	HB3	1.00	0.006	1.00	0.13
ARG30	HG2	1.00	0.006	1.00	0.11
ARG30	HG3	1.00	0.006	1.00	0.11
ARG30	H	1.00	0.006	1.00	-4695212.00
ARG30	HD2	0.87	0.002	1.00	0.06
ASP31	H	1.00	0.000	1.00	-147164.00
ASP31	HA	0.84	0.010	1.00	0.07

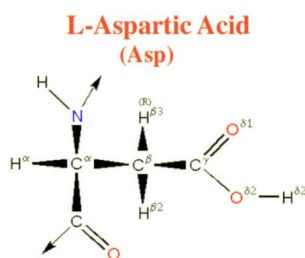
3.31 ASP(31)

Figure 30: Image from the BMRB

Residue probability: 0.857

Residue probability confidence: 0.893

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	175.282	176.463	2.348	0.000	0.000
CA 3.31.1	53.370	54.786	4.266	0.889	0.875
CB 3.31.2	42.722	40.949	3.070	0.833	0.833
N 3.31.3	121.895	120.550	5.690	0.860	1.000
HD2	NA	—	—	0.000	0.000
HA 3.31.4	5.210	4.587	0.329	0.750	0.875
HB2 3.31.5	2.467	2.708	0.282	1.000	0.833
HB3 3.31.6	2.468	2.654	0.285	1.000	0.833
H 3.31.7	8.377	8.304	1.027	0.670	1.000

3.31.1 Detailed Probabilities of ASP31CA:

Overall probability: 0.889

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG30	1.00	1.00
ASP31	0.75	0.80
VAL32	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R30HA	1.00
D31HD2	1.00
D31HB2	1.00
D31HB3	1.00
D31H	1.00
D31HA	1.00
V32H	1.00
V32HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG30	HA	1.00	0.009	1.00	0.06
ARG30	HB3	0.75	0.002	1.00	0.05
ARG30	H	0.84	0.010	1.00	0.07
ASP31	HA	1.00	0.003	1.00	3.52
ASP31	HB2	1.00	0.006	1.00	0.83
ASP31	HB3	1.00	0.005	1.00	0.83
ASP31	H	1.00	0.066	0.00	0.00
VAL32	HA	1.00	0.006	1.00	0.09
VAL32	H	1.00	0.002	1.00	1.35

3.31.2 Detailed Probabilities of ASP31CB:

Overall probability: 0.833

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP31	1.00	0.80
VAL32	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
D31HD2	1.00
D31HA	1.00
D31HB3	1.00
D31H	1.00
D31HB2	1.00
V32H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP31	HA	1.00	0.003	1.00	0.68
ASP31	HB2	1.00	0.006	1.00	7.31
ASP31	HB3	1.00	0.005	1.00	7.31
ASP31	H	1.00	0.014	1.00	0.60
VAL32	H	1.00	0.050	0.00	0.00
VAL32	HA	0.87	0.002	1.00	0.05

3.31.3 Detailed Probabilities of ASP31N:

Overall probability: 0.860

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG30	0.88	1.00
ASP31	1.00	1.00
VAL32	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
R30H	1.00
R30HA	1.00
R30HG3	0.96
R30HB3	1.00
R30HB2	1.00
R30HG2	0.98
D31HA	1.00
D31HB2	1.00
D31HB3	1.00
D31H	1.00
V32H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG30	HA	1.00	0.009	1.00	-2142537.00
ARG30	HB2	1.00	0.005	1.00	-486197.00
ARG30	HB3	1.00	0.004	1.00	-408723.00
ARG30	HG2	0.98	0.013	1.00	-408723.00
ARG30	HG3	0.96	0.058	0.04	0.00
ARG30	H	1.00	0.000	1.00	-147164.00
ARG30	HD2	0.58	0.003	1.00	-85905.00
ARG30	HD3	0.61	0.000	1.00	-113439.00
ASP31	HA	1.00	0.005	1.00	-542687.00
ASP31	HB2	1.00	0.002	1.00	-1309576.00
ASP31	HB3	1.00	0.001	1.00	-1309576.00
ASP31	H	1.00	0.006	1.00	-9420832.00
VAL32	H	1.00	0.058	0.00	0.00
VAL32	HA	0.91	0.009	1.00	-118246.00

3.31.4 Detailed Probabilities of ASP31HA:

Overall probability: 0.750

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG30	0.50	1.00
ASP31	1.00	0.80
VAL32	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
R30HA	1.00
D31HD2	1.00
D31HB2	1.00
D31HB3	1.00
D31H	1.00
D31HA	1.00
V32H	1.00
V32HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG30	HA	1.00	0.082	0.00	0.00
ARG30	H	0.84	0.001	1.00	-98556.00
ASP31	HA	1.00	0.003	1.00	3.52
ASP31	HB2	1.00	0.003	1.00	0.68
ASP31	HB3	1.00	0.003	1.00	0.68
ASP31	H	1.00	0.005	1.00	-542687.00
VAL32	HA	1.00	0.228	0.00	0.00
VAL32	H	1.00	0.003	1.00	-2249980.00

3.31.5 Detailed Probabilities of ASP31HB2:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP31	1.00	0.80
VAL32	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D31HD2	1.00
D31HA	1.00
D31HB3	1.00
D31H	1.00
D31HB2	1.00
V32H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP31	HA	1.00	0.005	1.00	0.83
ASP31	HB2	1.00	0.005	1.00	7.31
ASP31	HB3	1.00	0.005	1.00	7.31
ASP31	H	1.00	0.001	1.00	-1309576.00
VAL32	H	1.00	0.005	1.00	-527467.00
VAL32	HA	0.87	0.019	1.00	0.16

3.31.6 Detailed Probabilities of ASP31HB3:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP31	1.00	0.80
VAL32	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D31HD2	1.00
D31HA	1.00
D31HB2	1.00
D31H	1.00
D31HB3	1.00
V32H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP31	HA	1.00	0.005	1.00	0.83
ASP31	HB2	1.00	0.005	1.00	7.31
ASP31	HB3	1.00	0.005	1.00	7.31
ASP31	H	1.00	0.001	1.00	-1309576.00
VAL32	H	1.00	0.005	1.00	-527467.00
VAL32	HA	0.87	0.019	1.00	0.16

3.31.7 Detailed Probabilities of ASP31H:

Overall probability: 0.670

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG30	0.72	1.00
ASP31	0.75	1.00
VAL32	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R30H	1.00
R30HA	1.00
R30HG3	0.96
R30HB3	1.00
R30HB2	1.00
R30HG2	0.98
D31HA	1.00
D31HB2	1.00
D31HB3	1.00
D31H	1.00
V32H	1.00

NOESY contacts detailed probability

3.31 ASP(31)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG30	HA	1.00	0.043	0.00	0.00
ARG30	HB2	1.00	0.008	1.00	0.06
ARG30	HB3	1.00	0.003	1.00	0.11
ARG30	HG2	0.98	0.001	1.00	0.06
ARG30	HG3	0.96	0.556	0.04	0.00
ARG30	H	1.00	0.001	1.00	-120160.00
ARG30	HD2	0.58	0.007	1.00	0.08
ASP31	HA	1.00	0.066	0.00	0.00
ASP31	HB2	1.00	0.014	1.00	0.60
ASP31	HB3	1.00	0.014	1.00	0.60
ASP31	H	1.00	0.006	1.00	-9420832.00
VAL32	H	1.00	0.064	0.00	0.00

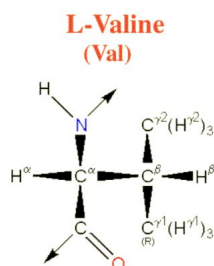
3.32 VAL(32)

Figure 31: Image from the BMRB

Residue probability: 0.792

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.114	175.682	2.367	0.000	0.000
CA 3.32.1	61.557	62.613	4.828	0.909	1.000
CB 3.32.2	33.884	32.918	4.591	0.571	1.000
CG1 3.32.3	21.735	21.563	2.746	0.833	1.000
CG2 3.32.4	21.142	21.368	2.801	0.800	1.000
N 3.32.5	120.426	121.057	5.832	0.909	1.000
HA 3.32.6	4.248	4.178	0.599	0.909	1.000
HB 3.32.7	1.776	1.980	0.322	0.857	1.000
HG1 3.32.8	0.867	0.816	0.264	1.000	1.000
HG2 3.32.9	0.763	0.803	0.504	0.400	1.000
H 3.32.10	8.441	8.311	0.669	0.727	1.000

3.32.1 Detailed Probabilities of VAL32CA:

Overall probability: 0.909

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP31	0.67	1.00
VAL32	1.00	1.00
ASN33	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D31HA	1.00
V32HG11	1.00
V32HG21	1.00
V32H	1.00
V32HB	1.00
V32HA	1.00
N33HA	1.00
N33H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP31	HA	1.00	0.228	0.00	0.00
ASP31	HB2	0.58	0.018	1.00	0.16
ASP31	HB3	0.87	0.019	1.00	0.16
VAL32	HA	1.00	0.005	1.00	3.85
VAL32	HB	1.00	0.001	1.00	0.28
VAL32	HG11	1.00	0.003	1.00	0.79
VAL32	HG21	1.00	0.002	1.00	0.84
VAL32	H	1.00	0.001	1.00	0.22
ASN33	HA	1.00	0.005	1.00	0.10
ASN33	H	1.00	0.006	1.00	1.16
ASN33	HB2	0.56	0.024	1.00	0.09

3.32.2 Detailed Probabilities of VAL32CB:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL32	0.40	1.00
ASN33	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
N33H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL32	HA	1.00	0.465	0.00	0.00
VAL32	HB	1.00	0.166	0.00	0.00
VAL32	HG11	1.00	0.001	1.00	1.38
VAL32	HG21	1.00	0.105	0.00	0.00
VAL32	H	1.00	0.001	1.00	0.45
ASN33	H	1.00	0.001	1.00	0.08
ASN33	HA	0.73	0.024	1.00	0.10

3.32.3 Detailed Probabilities of VAL32CG1:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL32	0.80	1.00
ASN33	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
N33H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL32	HA	1.00	0.009	1.00	1.04
VAL32	HB	1.00	0.001	1.00	2.08
VAL32	HG11	1.00	0.012	1.00	78.79
VAL32	HG21	1.00	0.346	0.00	0.00
VAL32	H	1.00	0.004	1.00	0.24
ASN33	H	0.97	0.006	1.00	0.34

3.32.4 Detailed Probabilities of VAL32CG2:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL32	0.80	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	0.004	1.00	1.02
VAL32	HB	1.00	0.003	1.00	1.63
VAL32	HG11	1.00	0.003	1.00	5.90
VAL32	HG21	1.00	0.101	0.00	0.00
VAL32	H	1.00	0.003	1.00	0.52

3.32.5 Detailed Probabilities of VAL32N:

Overall probability: 0.909

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP31	0.75	1.00
VAL32	1.00	1.00
ASN33	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D31HA	1.00
D31HB3	1.00
D31H	1.00
D31HB2	1.00
V32HA	1.00
V32HG11	1.00
V32HG21	1.00
V32HB	1.00
V32H	1.00
N33H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP31	HA	1.00	0.003	1.00	-2249980.00
ASP31	HB2	1.00	0.006	1.00	-527467.00
ASP31	HB3	1.00	0.005	1.00	-527467.00
ASP31	H	1.00	0.064	0.00	0.00
VAL32	HA	1.00	0.003	1.00	-455209.00
VAL32	HB	1.00	0.002	1.00	-802177.00
VAL32	HG11	1.00	0.004	1.00	-408285.00
VAL32	HG21	1.00	0.014	1.00	-867899.00
VAL32	H	1.00	0.000	1.00	-7356552.00
ASN33	H	1.00	0.009	1.00	-142388.00
ASN33	HA	0.82	0.026	1.00	-276726.00

3.32.6 Detailed Probabilities of VAL32HA:

Overall probability: 0.909

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP31	1.00	1.00
VAL32	0.80	1.00
ASN33	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D31HA	1.00
V32HG11	1.00
V32HG21	1.00
V32H	1.00
V32HB	1.00
V32HA	1.00
N33HA	1.00
N33H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP31	HA	1.00	0.006	1.00	0.09
ASP31	HB2	0.58	0.002	1.00	0.05
ASP31	HB3	0.87	0.002	1.00	0.05
ASP31	H	0.91	0.009	1.00	-118246.00
VAL32	HA	1.00	0.005	1.00	3.85
VAL32	HB	1.00	0.465	0.00	0.00
VAL32	HG11	1.00	0.009	1.00	1.04
VAL32	HG21	1.00	0.004	1.00	1.02
VAL32	H	1.00	0.003	1.00	-455209.00
ASN33	HA	1.00	0.008	1.00	0.20
ASN33	H	1.00	0.003	1.00	-1976566.00

3.32.7 Detailed Probabilities of VAL32HB:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL32	0.80	1.00
ASN33	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
N33H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL32	HA	1.00	0.001	1.00	0.28
VAL32	HB	1.00	0.166	0.00	0.00
VAL32	HG11	1.00	0.001	1.00	2.08
VAL32	HG21	1.00	0.003	1.00	1.63
VAL32	H	1.00	0.002	1.00	-802177.00
ASN33	H	1.00	0.010	1.00	-125025.00
ASN33	HA	0.73	0.006	1.00	0.19

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
ASN33	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
N33H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL32	HA	1.00	0.003	1.00	0.79
VAL32	HB	1.00	0.001	1.00	1.38
VAL32	HG11	1.00	0.012	1.00	78.79
VAL32	HG21	1.00	0.003	1.00	5.90
VAL32	H	1.00	0.004	1.00	-408285.00
ASN33	H	0.97	0.001	1.00	-477045.00
ASN33	HA	0.54	0.009	1.00	0.35

3.32.9 Detailed Probabilities of VAL32HG21:

Overall probability: 0.400

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL32	0.40	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	0.002	1.00	0.84
VAL32	HB	1.00	0.105	0.00	0.00
VAL32	HG11	1.00	0.346	0.00	0.00
VAL32	HG21	1.00	0.101	0.00	0.00
VAL32	H	1.00	0.014	1.00	-867899.00

3.32.10 Detailed Probabilities of VAL32H:

Overall probability: 0.727

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP31	0.25	1.00
VAL32	1.00	1.00
ASN33	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D31HA	1.00
D31HB3	1.00
D31H	1.00
D31HB2	1.00
V32HA	1.00
V32HG11	1.00
V32HG21	1.00
V32HB	1.00
V32H	1.00
N33H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP31	HA	1.00	0.002	1.00	1.35
ASP31	HB2	1.00	0.050	0.00	0.00
ASP31	HB3	1.00	0.050	0.00	0.00
ASP31	H	1.00	0.058	0.00	0.00
VAL32	HA	1.00	0.001	1.00	0.22
VAL32	HB	1.00	0.001	1.00	0.45
VAL32	HG11	1.00	0.004	1.00	0.24
VAL32	HG21	1.00	0.003	1.00	0.52
VAL32	H	1.00	0.000	1.00	-7356552.00
ASN33	H	1.00	0.005	1.00	-158315.00
ASN33	HA	0.82	0.023	1.00	0.30

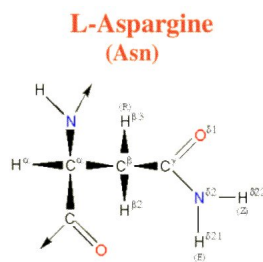
3.33 ASN(33)

Figure 32: Image from the BMRB

Residue probability: 0.789
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.235	175.315	1.862	0.000	0.000
CA 3.33.1	53.396	53.674	5.429	0.667	1.000
CB 3.33.2	40.869	38.785	5.449	0.571	1.000
N 3.33.3	122.700	118.907	6.480	1.000	1.000
ND2 3.33.4	114.609	112.932	14.355	1.000	1.000
HA 3.33.5	4.977	4.658	0.371	0.727	1.000
HB2 3.33.6	2.910	2.800	0.341	0.571	1.000
HB3 3.33.7	2.689	2.739	0.364	0.857	1.000
H 3.33.8	9.550	8.328	0.633	0.833	1.000
HD21 3.33.9	7.938	7.343	1.188	1.000	1.000
HD22 3.33.10	7.020	7.145	1.184	0.667	1.000

3.33.1 Detailed Probabilities of ASN33CA:

Overall probability: 0.667
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL32	1.00	1.00
ASN33	0.50	1.00
ASP34	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
V32HA	1.00
N33HB2	1.00
N33HB3	1.00
N33H	1.00
N33HD21	1.00
N33HD22	1.00
N33HA	1.00
D34HA	1.00
D34H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL32	HA	1.00	0.008	1.00	0.20
VAL32	HB	0.73	0.006	1.00	0.19
VAL32	HG11	0.56	0.009	1.00	0.35
VAL32	H	0.82	0.023	1.00	0.30
ASN33	HA	1.00	0.003	1.00	6.28
ASN33	HB2	1.00	0.222	0.00	0.00
ASN33	HB3	1.00	0.004	1.00	0.54
ASN33	H	1.00	0.069	0.00	0.00
ASN33	HD21	1.00	0.021	1.00	0.09
ASN33	HD22	1.00	0.155	0.00	0.00
ASP34	HA	1.00	0.200	0.00	0.00
ASP34	H	1.00	0.019	1.00	0.29

3.33.2 Detailed Probabilities of ASN33CB:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN33	0.50	1.00
ASP34	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N33HA	1.00
N33HB2	1.00
N33H	1.00
N33HD21	1.00
N33HD22	1.00
N33HB3	1.00
D34H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN33	HA	1.00	0.448	0.00	0.00
ASN33	HB2	1.00	0.065	0.00	0.00
ASN33	HB3	1.00	0.156	0.00	0.00
ASN33	H	1.00	0.006	1.00	0.50
ASN33	HD21	1.00	0.004	1.00	0.60
ASN33	HD22	1.00	0.002	1.00	0.28
ASP34	H	1.00	0.003	1.00	0.19

3.33.3 Detailed Probabilities of ASN33N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL32	1.00	1.00
ASN33	1.00	1.00
ASP34	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V32H	1.00
V32HG13	0.96
V32HB	1.00
V32HA	1.00
N33HA	1.00
N33HB2	1.00
N33HB3	1.00
N33HD21	0.98
N33H	1.00
D34H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL32	HA	1.00	0.003	1.00	-1976566.00
VAL32	HB	1.00	0.010	1.00	-125025.00
VAL32	HG11	0.98	0.001	1.00	-477045.00
VAL32	H	1.00	0.005	1.00	-158315.00
VAL32	HG21	0.94	0.008	1.00	-447116.00
ASN33	HA	1.00	0.002	1.00	-452028.00
ASN33	HB2	1.00	0.002	1.00	-465560.00
ASN33	HB3	1.00	0.005	1.00	-782777.00
ASN33	H	1.00	0.006	1.00	-5172523.00
ASN33	HD21	0.98	0.006	1.00	-216616.00
ASN33	HD22	0.63	0.001	1.00	-124030.00
ASP34	H	1.00	0.003	1.00	-1416699.00
ASP34	HB2	0.57	0.003	1.00	-465560.00

3.33.4 Detailed Probabilities of ASN33ND2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN33	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N33HA	1.00
N33HB2	1.00
N33HB3	1.00
N33H	0.98
N33HD22	1.00
N33HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN33	HA	1.00	0.000	1.00	-167027.00
ASN33	HB2	1.00	0.005	1.00	-500827.00
ASN33	HB3	1.00	0.002	1.00	-732739.00
ASN33	H	0.98	0.004	1.00	-191521.00
ASN33	HD21	1.00	0.006	1.00	-6493433.00
ASN33	HD22	1.00	0.005	1.00	-5275216.00

3.33.5 Detailed Probabilities of ASN33HA:

Overall probability: 0.727

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL32	1.00	1.00
ASN33	0.67	1.00
ASP34	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
V32HA	1.00
N33HB2	1.00
N33HB3	1.00
N33H	1.00
N33HD21	1.00
N33HD22	1.00
N33HA	1.00
D34HA	1.00
D34H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL32	HA	1.00	0.005	1.00	0.10
VAL32	HB	0.73	0.024	1.00	0.10
VAL32	H	0.82	0.026	1.00	-276726.00
ASN33	HA	1.00	0.003	1.00	6.28
ASN33	HB2	1.00	1.775	0.00	0.00
ASN33	HB3	1.00	0.448	0.00	0.00
ASN33	H	1.00	0.002	1.00	-452028.00
ASN33	HD21	1.00	0.000	1.00	-167027.00
ASN33	HD22	1.00	0.006	1.00	-129700.00
ASP34	HA	1.00	0.124	0.00	0.00
ASP34	H	1.00	0.003	1.00	-446570.00

3.33.6 Detailed Probabilities of ASN33HB2:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN33	0.50	1.00
ASP34	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N33HA	1.00
N33HB3	1.00
N33H	1.00
N33HD21	1.00
N33HD22	1.00
N33HB2	1.00
D34H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN33	HA	1.00	0.222	0.00	0.00
ASN33	HB2	1.00	0.221	0.00	0.00
ASN33	HB3	1.00	0.065	0.00	0.00
ASN33	H	1.00	0.002	1.00	-465560.00
ASN33	HD21	1.00	0.005	1.00	-500827.00
ASN33	HD22	1.00	0.001	1.00	-497036.00
ASP34	H	1.00	0.003	1.00	-495541.00

3.33.7 Detailed Probabilities of ASN33HB3:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN33	0.83	1.00
ASP34	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N33HA	1.00
N33HB2	1.00
N33H	1.00
N33HD21	1.00
N33HD22	1.00
N33HB3	1.00
D34H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN33	HA	1.00	0.004	1.00	0.54
ASN33	HB2	1.00	0.000	1.00	3.06
ASN33	HB3	1.00	0.156	0.00	0.00
ASN33	H	1.00	0.005	1.00	-782777.00
ASN33	HD21	1.00	0.002	1.00	-732739.00
ASN33	HD22	1.00	0.001	1.00	-459579.00
ASP34	H	1.00	0.016	1.00	-407707.00

3.33.8 Detailed Probabilities of ASN33H:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL32	1.00	1.00
ASN33	0.67	1.00
ASP34	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V32H	1.00
V32HG13	0.96
V32HB	1.00
V32HA	1.00
N33HA	1.00
N33HB2	1.00
N33HB3	1.00
N33HD21	0.98
N33H	1.00
D34H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL32	HA	1.00	0.006	1.00	1.16
VAL32	HB	1.00	0.001	1.00	0.08
VAL32	HG11	0.98	0.006	1.00	0.34
VAL32	H	1.00	0.009	1.00	-142388.00
VAL32	HG21	0.94	0.001	1.00	0.19
ASN33	HA	1.00	0.069	0.00	0.00
ASN33	HB2	1.00	0.867	0.00	0.00
ASN33	HB3	1.00	0.006	1.00	0.50
ASN33	H	1.00	0.006	1.00	-5172523.00
ASN33	HD21	0.98	0.004	1.00	-191521.00
ASN33	HD22	0.63	0.003	1.00	-160323.00
ASP34	H	1.00	0.007	1.00	-1695837.00

3.33.9 Detailed Probabilities of ASN33HD21:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN33	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N33HA	1.00
N33HB2	1.00
N33HB3	1.00
N33H	0.98
N33HD22	1.00
N33HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN33	HA	1.00	0.021	1.00	0.09
ASN33	HB2	1.00	0.006	1.00	0.47
ASN33	HB3	1.00	0.004	1.00	0.60
ASN33	H	0.98	0.006	1.00	-216616.00
ASN33	HD21	1.00	0.006	1.00	-6493433.00
ASN33	HD22	1.00	0.003	1.00	-5684875.00

3.33.10 Detailed Probabilities of ASN33HD22:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN33	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
N33HA	1.00
N33HB2	1.00
N33HB3	1.00
N33HD21	1.00
N33HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN33	HA	1.00	0.155	0.00	0.00
ASN33	HB2	1.00	0.268	0.00	0.00
ASN33	HB3	1.00	0.002	1.00	0.28
ASN33	HD21	1.00	0.005	1.00	-5275216.00
ASN33	HD22	1.00	0.013	1.00	-22611540.00
ASN33	H	0.63	0.001	1.00	-124030.00

3.34 ASP(34)

Figure 33: Image from the BMRB

Residue probability: 0.750

Residue probability confidence: 0.893

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	175.626	176.463	2.348	0.000	0.000
CA 3.34.1	53.483	54.786	4.266	0.500	0.875
CB 3.34.2	42.396	40.949	3.070	0.800	0.833
N 3.34.3	114.885	120.550	5.690	1.000	1.000
HD2	NA	—	—	0.000	0.000
HA 3.34.4	4.703	4.587	0.329	0.714	0.875
HB2 3.34.5	2.909	2.708	0.282	0.800	0.833
HB3 3.34.6	3.086	2.654	0.285	0.600	0.833
H 3.34.7	7.616	8.304	1.027	0.833	1.000

3.34.1 Detailed Probabilities of ASP34CA:

Overall probability: 0.500

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN33	0.00	1.00
ASP34	0.63	0.80
SER35	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
N33HA	1.00
D34HD2	1.00
D34HB2	1.00
D34HB3	1.00
D34H	1.00
D34HA	1.00
S35H	1.00
S35HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN33	HA	1.00	0.124	0.00	0.00
ASP34	HA	1.00	0.011	1.00	10.60
ASP34	HB2	1.00	0.191	0.00	0.00
ASP34	HB3	1.00	0.014	1.00	0.90
ASP34	H	1.00	0.035	0.50	0.00
SER35	HA	1.00	0.063	0.00	0.00
SER35	H	1.00	0.008	1.00	0.78

3.34.2 Detailed Probabilities of ASP34CB:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP34	0.75	0.80
SER35	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D34HD2	1.00
D34HA	1.00
D34HB3	1.00
D34H	1.00
D34HB2	1.00
S35H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP34	HA	1.00	0.002	1.00	0.79
ASP34	HB2	1.00	0.008	1.00	220.78
ASP34	HB3	1.00	0.813	0.00	0.00
ASP34	H	1.00	0.011	1.00	0.26
SER35	H	1.00	0.005	1.00	0.28

3.34.3 Detailed Probabilities of ASP34N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN33	1.00	1.00
ASP34	1.00	1.00
SER35	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N33HB3	1.00
N33HB2	1.00
N33HA	1.00
N33H	1.00
D34HA	1.00
D34HB2	1.00
D34HB3	1.00
D34H	1.00
S35H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN33	HA	1.00	0.003	1.00	-446570.00
ASN33	HB2	1.00	0.003	1.00	-495541.00
ASN33	HB3	1.00	0.016	1.00	-407707.00
ASN33	H	1.00	0.007	1.00	-1695837.00
ASP34	HA	1.00	0.001	1.00	-570196.00
ASP34	HB2	1.00	0.004	1.00	-495541.00
ASP34	HB3	1.00	0.001	1.00	-207209.00
ASP34	H	1.00	0.002	1.00	-11429987.00
SER35	H	1.00	0.010	1.00	-90754.00
SER35	HA	0.84	0.026	1.00	-156276.00

3.34.4 Detailed Probabilities of ASP34HA:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN33	0.00	1.00
ASP34	1.00	0.80
SER35	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
N33HA	1.00
D34HD2	1.00
D34HB2	1.00
D34HB3	1.00
D34H	1.00
D34HA	1.00
S35H	1.00
S35HA	1.00

NOESY contacts detailed probability

3.34 ASP(34)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN33	HA	1.00	0.200	0.00	0.00
ASP34	HA	1.00	0.011	1.00	10.60
ASP34	HB2	1.00	0.002	1.00	0.79
ASP34	HB3	1.00	0.005	1.00	0.64
ASP34	H	1.00	0.001	1.00	-570196.00
SER35	HA	1.00	2.457	0.00	0.00
SER35	H	1.00	0.003	1.00	-979840.00

3.34.5 Detailed Probabilities of ASP34HB2:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP34	0.75	0.80
SER35	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D34HD2	1.00
D34HA	1.00
D34HB3	1.00
D34H	1.00
D34HB2	1.00
S35H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP34	HA	1.00	0.191	0.00	0.00
ASP34	HB2	1.00	0.008	1.00	220.78
ASP34	HB3	1.00	0.002	1.00	2.15
ASP34	H	1.00	0.004	1.00	-495541.00
SER35	H	1.00	0.002	1.00	-601808.00

3.34.6 Detailed Probabilities of ASP34HB3:

Overall probability: 0.600

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP34	0.50	0.80
SER35	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D34HD2	1.00
D34HA	1.00
D34HB2	1.00
D34H	1.00
D34HB3	1.00
S35H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP34	HA	1.00	0.014	1.00	0.90
ASP34	HB2	1.00	0.813	0.00	0.00
ASP34	HB3	1.00	0.175	0.00	0.00
ASP34	H	1.00	0.001	1.00	-207209.00
SER35	H	1.00	0.003	1.00	-865116.00

3.34.7 Detailed Probabilities of ASP34H:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN33	0.75	1.00
ASP34	0.87	1.00
SER35	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N33HB3	1.00
N33HB2	1.00
N33HA	1.00
N33H	1.00
D34HA	1.00
D34HB2	1.00
D34HB3	1.00
D34H	1.00
S35H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN33	HA	1.00	0.019	1.00	0.29
ASN33	HB2	1.00	0.328	0.00	0.00
ASN33	HB3	1.00	0.003	1.00	0.19
ASN33	H	1.00	0.003	1.00	-1416699.00
ASP34	HA	1.00	0.035	0.50	0.00
ASP34	HB2	1.00	0.011	1.00	0.26
ASP34	HB3	1.00	0.018	1.00	0.10
ASP34	H	1.00	0.002	1.00	-11429987.00
SER35	H	1.00	0.019	1.00	-111496.00

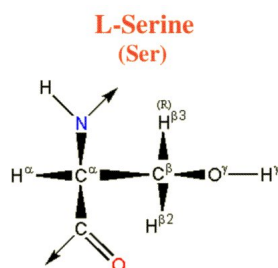
3.35 SER(35)

Figure 34: Image from the BMRB

Residue probability: 0.691

Residue probability confidence: 0.864

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	175.991	174.682	1.868	0.000	0.000
CA 3.35.1	61.446	58.750	3.025	0.000	0.875
CB 3.35.2	62.764	63.523	4.288	0.833	0.833
N 3.35.3	114.381	116.135	5.326	1.000	0.900
HA 3.35.4	4.046	4.486	0.430	0.500	0.875
HB2 3.35.5	3.919	3.856	0.325	0.800	0.833
HB3 3.35.6	3.949	3.825	0.343	0.800	0.833
H 3.35.7	8.869	8.292	0.600	0.900	0.900
HG	NA	—	—	0.000	0.000

3.35.1 Detailed Probabilities of SER35CA:

Overall probability: 0.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP34	0.00	1.00
SER35	0.00	0.80
ASP36	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D34HA	1.00
S35HB2	1.00
S35HB3	1.00
S35H	1.00
S35HG	1.00
S35HA	1.00
D36HA	1.00
D36H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP34	HA	1.00	2.457	0.00	0.00
SER35	HA	1.00	1.800	0.00	0.00
SER35	HB2	1.00	1.673	0.00	0.00
SER35	HB3	1.00	1.703	0.00	0.00
SER35	H	1.00	0.136	0.00	0.00
ASP36	HA	1.00	2.273	0.00	0.00
ASP36	H	1.00	0.617	0.00	0.00

3.35.2 Detailed Probabilities of SER35CB:

Overall probability: 0.833

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
SER35	0.75	0.80
ASP36	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S35HA	1.00
S35HB2	1.00
S35H	1.00
S35HG	1.00
S35HB3	1.00
D36H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER35	HA	1.00	0.108	0.00	0.00
SER35	HB2	1.00	0.019	1.00	14.42
SER35	HB3	1.00	0.011	1.00	14.42
SER35	H	1.00	0.003	1.00	0.45
ASP36	H	1.00	0.011	1.00	0.20
ASP36	HA	0.71	0.004	1.00	0.05

3.35.3 Detailed Probabilities of SER35N:

Overall probability: 1.000

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP34	1.00	1.00
SER35	1.00	0.80
ASP36	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D34H	1.00
D34HB2	1.00
D34HA	1.00
D34HB3	1.00
S35HA	1.00
S35HB2	1.00
S35HB3	1.00
S35HG	1.00
S35H	1.00
D36H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP34	HA	1.00	0.003	1.00	-979840.00
ASP34	HB2	1.00	0.002	1.00	-601808.00
ASP34	HB3	1.00	0.003	1.00	-865116.00
ASP34	H	1.00	0.019	1.00	-111496.00
SER35	HA	1.00	0.001	1.00	-523841.00
SER35	HB2	1.00	0.015	1.00	-1028804.00
SER35	HB3	1.00	0.015	1.00	-1028804.00
SER35	H	1.00	0.003	1.00	-3412426.00
ASP36	H	1.00	0.010	1.00	-545988.00

3.35.4 Detailed Probabilities of SER35HA:

Overall probability: 0.500

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP34	0.50	1.00
SER35	0.25	0.80
ASP36	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D34HA	1.00
S35HB2	1.00
S35HB3	1.00
S35H	1.00
S35HG	1.00
S35HA	1.00
D36HA	1.00
D36H	1.00

NOESY contacts detailed probability

3.35 SER(35)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP34	HA	1.00	0.063	0.00	0.00
ASP34	H	0.84	0.026	1.00	-156276.00
SER35	HA	1.00	1.800	0.00	0.00
SER35	HB2	1.00	0.108	0.00	0.00
SER35	HB3	1.00	0.108	0.00	0.00
SER35	H	1.00	0.001	1.00	-523841.00
ASP36	HA	1.00	0.007	1.00	0.20
ASP36	H	1.00	0.009	1.00	-392761.00

3.35.5 Detailed Probabilities of SER35HB2:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
SER35	0.75	0.80
ASP36	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S35HA	1.00
S35HB3	1.00
S35H	1.00
S35HG	1.00
S35HB2	1.00
D36H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER35	HA	1.00	1.673	0.00	0.00
SER35	HB2	1.00	0.019	1.00	14.42
SER35	HB3	1.00	0.019	1.00	14.42
SER35	H	1.00	0.015	1.00	-1028804.00
ASP36	H	1.00	0.018	1.00	-454936.00

3.35.6 Detailed Probabilities of SER35HB3:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
SER35	0.75	0.80
ASP36	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S35HA	1.00
S35HB2	1.00
S35H	1.00
S35HG	1.00
S35HB3	1.00
D36H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER35	HA	1.00	1.703	0.00	0.00
SER35	HB2	1.00	0.011	1.00	14.42
SER35	HB3	1.00	0.011	1.00	14.42
SER35	H	1.00	0.015	1.00	-1028804.00
ASP36	H	1.00	0.012	1.00	-454936.00

3.35.7 Detailed Probabilities of SER35H:

Overall probability: 0.900

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP34	1.00	1.00
SER35	0.75	0.80
ASP36	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D34H	1.00
D34HB2	1.00
D34HA	1.00
D34HB3	1.00
S35HA	1.00
S35HB2	1.00
S35HB3	1.00
S35HG	1.00
S35H	1.00
D36H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP34	HA	1.00	0.008	1.00	0.78
ASP34	HB2	1.00	0.005	1.00	0.28
ASP34	HB3	1.00	0.002	1.00	0.44
ASP34	H	1.00	0.010	1.00	-90754.00
SER35	HA	1.00	0.136	0.00	0.00
SER35	HB2	1.00	0.003	1.00	0.45
SER35	HB3	1.00	0.003	1.00	0.45
SER35	H	1.00	0.003	1.00	-3412426.00
ASP36	H	1.00	0.004	1.00	-444346.00
ASP36	HA	0.83	0.010	1.00	0.09

3.36 ASP(36)

Figure 35: Image from the BMRB

Residue probability: 0.884

Residue probability confidence: 0.864

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	179.136	176.463	2.348	0.000	0.000
CA 3.36.1	57.668	54.786	4.266	1.000	0.875
CB 3.36.2	40.284	40.949	3.070	0.833	0.833
N 3.36.3	124.695	120.550	5.690	1.000	0.900
HD2	NA	—	—	0.000	0.000
HA 3.36.4	4.519	4.587	0.329	0.889	0.875
HB2 3.36.5	2.842	2.708	0.282	1.000	0.833
HB3 3.36.6	2.662	2.654	0.285	0.667	0.833
H 3.36.7	8.388	8.304	1.027	0.800	0.900

3.36.1 Detailed Probabilities of ASP36CA:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
SER35	1.00	1.00
ASP36	1.00	0.80
GLU37	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S35HA	1.00
D36HD2	1.00
D36HB2	1.00
D36HB3	1.00
D36H	1.00
D36HA	1.00
E37H	1.00
E37HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER35	HA	1.00	0.007	1.00	0.20
SER35	H	0.83	0.010	1.00	0.09
ASP36	HA	1.00	0.012	1.00	10.70
ASP36	HB2	1.00	0.009	1.00	0.84
ASP36	HB3	1.00	0.007	1.00	1.29
ASP36	H	1.00	0.007	1.00	0.57
GLU37	HA	1.00	0.006	1.00	0.20
GLU37	H	1.00	0.004	1.00	0.20

3.36.2 Detailed Probabilities of ASP36CB:

Overall probability: 0.833

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP36	0.75	0.80
GLU37	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D36HD2	1.00
D36HA	1.00
D36HB3	1.00
D36H	1.00
D36HB2	1.00
E37H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP36	HA	1.00	0.011	1.00	1.02
ASP36	HB2	1.00	0.006	1.00	6.23
ASP36	HB3	1.00	0.007	1.00	6.23
ASP36	H	1.00	0.627	0.00	0.00
GLU37	H	1.00	0.006	1.00	0.62
GLU37	HA	0.54	0.003	1.00	0.08

3.36.3 Detailed Probabilities of ASP36N:

Overall probability: 1.000

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
SER35	1.00	0.80
ASP36	1.00	1.00
GLU37	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S35HB2	1.00
S35H	1.00
S35HA	1.00
S35HG	0.97
S35HB3	1.00
D36HA	1.00
D36HB2	1.00
D36HB3	1.00
D36H	1.00
E37H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER35	HA	1.00	0.009	1.00	-392761.00
SER35	HB2	1.00	0.018	1.00	-454936.00
SER35	HB3	1.00	0.012	1.00	-454936.00
SER35	H	1.00	0.004	1.00	-444346.00
ASP36	HA	1.00	0.011	1.00	-1042027.00
ASP36	HB2	1.00	0.009	1.00	-1705772.00
ASP36	HB3	1.00	0.007	1.00	-1061847.00
ASP36	H	1.00	0.007	1.00	-9750438.00
GLU37	H	1.00	0.003	1.00	-1787374.00
GLU37	HA	0.86	0.004	1.00	-392761.00
GLU37	HB2	0.58	0.020	1.00	-76025.00

3.36.4 Detailed Probabilities of ASP36HA:

Overall probability: 0.889

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
SER35	0.67	1.00
ASP36	1.00	0.80
GLU37	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S35HA	1.00
D36HD2	1.00
D36HB2	1.00
D36HB3	1.00
D36H	1.00
D36HA	1.00
E37H	1.00
E37HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER35	HA	1.00	2.273	0.00	0.00
SER35	HB2	0.65	0.004	1.00	0.05
SER35	HB3	0.71	0.004	1.00	0.05
ASP36	HA	1.00	0.012	1.00	10.70
ASP36	HB2	1.00	0.011	1.00	1.02
ASP36	HB3	1.00	0.010	1.00	1.38
ASP36	H	1.00	0.011	1.00	-1042027.00
GLU37	HA	1.00	0.013	1.00	0.08
GLU37	H	1.00	0.011	1.00	-296991.00

3.36.5 Detailed Probabilities of ASP36HB2:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP36	1.00	0.80
GLU37	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D36HD2	1.00
D36HA	1.00
D36HB3	1.00
D36H	1.00
D36HB2	1.00
E37H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP36	HA	1.00	0.009	1.00	0.84
ASP36	HB2	1.00	0.006	1.00	6.23
ASP36	HB3	1.00	0.003	1.00	6.13
ASP36	H	1.00	0.009	1.00	-1705772.00
GLU37	H	1.00	0.006	1.00	-696957.00

3.36.6 Detailed Probabilities of ASP36HB3:

Overall probability: 0.667

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP36	0.75	0.80
GLU37	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
D36HD2	1.00
D36HA	1.00
D36HB2	1.00
D36H	1.00
D36HB3	1.00
E37H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP36	HA	1.00	0.007	1.00	1.29
ASP36	HB2	1.00	0.007	1.00	6.23
ASP36	HB3	1.00	0.183	0.00	0.00
ASP36	H	1.00	0.007	1.00	-1061847.00
GLU37	H	1.00	0.056	0.00	0.00
GLU37	HA	0.84	0.019	1.00	0.09

3.36.7 Detailed Probabilities of ASP36H:

Overall probability: 0.800

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
SER35	0.75	0.80
ASP36	0.75	1.00
GLU37	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S35HB2	1.00
S35H	1.00
S35HA	1.00
S35HG	0.97
S35HB3	1.00
D36HA	1.00
D36HB2	1.00
D36HB3	1.00
D36H	1.00
E37H	1.00

NOESY contacts detailed probability

3.36 ASP(36)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER35	HA	1.00	0.617	0.00	0.00
SER35	HB2	1.00	0.011	1.00	0.20
SER35	HB3	1.00	0.011	1.00	0.20
SER35	H	1.00	0.010	1.00	-545988.00
ASP36	HA	1.00	0.007	1.00	0.57
ASP36	HB2	1.00	0.627	0.00	0.00
ASP36	HB3	1.00	0.011	1.00	0.80
ASP36	H	1.00	0.007	1.00	-9750438.00
GLU37	H	1.00	0.004	1.00	-1289255.00
GLU37	HA	0.86	0.012	1.00	0.35

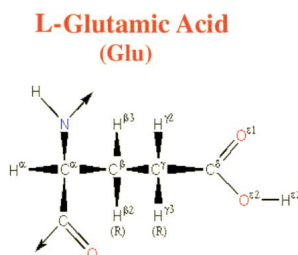


Figure 36: Image from the BMRB

Residue probability: 0.842
Residue probability confidence: 0.925

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.698	176.942	2.547	0.000	0.000
CA 3.37.1	59.209	57.442	3.837	0.873	1.000
CB 3.37.2	29.721	30.185	4.018	0.714	0.875
CG 3.37.3	36.545	36.085	1.533	1.000	0.875
N 3.37.4	122.449	120.574	4.837	0.917	1.000
HA 3.37.5	4.059	4.245	0.429	0.909	1.000
HB2 3.37.6	2.269	2.021	0.233	0.571	0.875
HB3 3.37.7	2.175	1.994	0.244	0.714	0.875
HG2 3.37.8	2.442	2.258	0.226	0.859	0.875
HG3 3.37.9	2.728	2.233	0.232	0.861	0.875
H 3.37.10	9.009	8.332	0.601	1.000	1.000
HE2	NA	—	—	0.000	0.000

3.37.1 Detailed Probabilities of GLU37CA:

Overall probability: 0.873
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP36	1.00	1.00
GLU37	1.00	1.00
LEU38	0.30	1.00

Expected NOESY Contacts

Proton	Expected probability
D36HA	1.00
E37HB2	1.00
E37HB3	1.00
E37HG2	1.00
E37HG3	1.00
E37H	1.00
E37HA	1.00
L38H	1.00
L38HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP36	HA	1.00	0.013	1.00	0.08
ASP36	HB3	0.84	0.019	1.00	0.09
ASP36	H	0.86	0.012	1.00	0.35
GLU37	HA	1.00	0.017	1.00	41.95
GLU37	HB2	1.00	0.013	1.00	2.14
GLU37	HB3	1.00	0.010	1.00	2.61
GLU37	HG2	1.00	0.018	1.00	1.54
GLU37	HG3	1.00	0.004	1.00	0.36
GLU37	H	1.00	0.002	1.00	0.46
LEU38	HA	1.00	0.098	0.00	0.00
LEU38	H	1.00	0.034	0.60	0.00

3.37.2 Detailed Probabilities of GLU37CB:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU37	0.67	0.86
LEU38	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E37HA	1.00
E37HB3	1.00
E37HG2	1.00
E37HG3	1.00
E37H	1.00
E37HE2	1.00
E37HB2	1.00
L38H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU37	HA	1.00	0.012	1.00	0.50
GLU37	HB2	1.00	0.174	0.00	0.00
GLU37	HB3	1.00	0.268	0.00	0.00
GLU37	HG2	1.00	0.001	1.00	0.60
GLU37	HG3	1.00	0.002	1.00	0.40
GLU37	H	1.00	0.004	1.00	0.38
LEU38	H	1.00	0.010	1.00	0.20

3.37.3 Detailed Probabilities of GLU37CG:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU37	1.00	0.86
LEU38	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E37HA	1.00
E37HB2	1.00
E37HB3	1.00
E37HG3	1.00
E37H	1.00
E37HE2	1.00
E37HG2	1.00
L38H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU37	HA	1.00	0.006	1.00	1.15
GLU37	HB2	1.00	0.014	1.00	6.47
GLU37	HB3	1.00	0.003	1.00	2.93
GLU37	HG2	1.00	0.003	1.00	35.10
GLU37	HG3	1.00	0.000	1.00	4.17
GLU37	H	1.00	0.004	1.00	0.43
LEU38	H	0.98	0.026	1.00	0.08

3.37.4 Detailed Probabilities of GLU37N:

Overall probability: 0.917

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP36	0.75	1.00
GLU37	1.00	1.00
LEU38	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D36H	1.00
D36HA	1.00
D36HB3	1.00
D36HB2	1.00
E37HA	1.00
E37HB2	1.00
E37HB3	1.00
E37HG2	1.00
E37HG3	1.00
E37H	1.00
L38H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP36	HA	1.00	0.011	1.00	-296991.00
ASP36	HB2	1.00	0.006	1.00	-696957.00
ASP36	HB3	1.00	0.056	0.00	0.00
ASP36	H	1.00	0.004	1.00	-1289255.00
GLU37	HA	1.00	0.014	1.00	-737943.00
GLU37	HB2	1.00	0.000	1.00	-516897.00
GLU37	HB3	1.00	0.005	1.00	-842467.00
GLU37	HG2	1.00	0.003	1.00	-484121.00
GLU37	HG3	1.00	0.010	1.00	-889219.00
GLU37	H	1.00	0.003	1.00	-6948421.00
LEU38	H	1.00	0.007	1.00	-760971.00
LEU38	HA	0.93	0.015	1.00	-108913.00

3.37.5 Detailed Probabilities of GLU37HA:

Overall probability: 0.909

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP36	1.00	1.00
GLU37	1.00	1.00
LEU38	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
D36HA	1.00
E37HB2	1.00
E37HB3	1.00
E37HG2	1.00
E37HG3	1.00
E37H	1.00
E37HA	1.00
L38H	1.00
L38HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP36	HA	1.00	0.006	1.00	0.20
ASP36	HB2	0.54	0.003	1.00	0.08
ASP36	H	0.86	0.004	1.00	-392761.00
GLU37	HA	1.00	0.017	1.00	41.95
GLU37	HB2	1.00	0.012	1.00	0.50
GLU37	HB3	1.00	0.004	1.00	1.52
GLU37	HG2	1.00	0.006	1.00	1.15
GLU37	HG3	1.00	0.013	1.00	0.57
GLU37	H	1.00	0.014	1.00	-737943.00
LEU38	HA	1.00	0.140	0.00	0.00
LEU38	H	1.00	0.005	1.00	-580741.00

3.37.6 Detailed Probabilities of GLU37HB2:

Overall probability: 0.571

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU37	0.67	0.86
LEU38	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E37HA	1.00
E37HB3	1.00
E37HG2	1.00
E37HG3	1.00
E37H	1.00
E37HE2	1.00
E37HB2	1.00
L38H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU37	HA	1.00	0.013	1.00	2.14
GLU37	HB2	1.00	0.174	0.00	0.00
GLU37	HB3	1.00	0.087	0.00	0.00
GLU37	HG2	1.00	0.014	1.00	6.47
GLU37	HG3	1.00	0.012	1.00	0.78
GLU37	H	1.00	0.000	1.00	-516897.00
LEU38	H	1.00	0.140	0.00	0.00

3.37.7 Detailed Probabilities of GLU37HB3:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU37	0.83	0.86
LEU38	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E37HA	1.00
E37HB2	1.00
E37HG2	1.00
E37HG3	1.00
E37H	1.00
E37HE2	1.00
E37HB3	1.00
L38H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU37	HA	1.00	0.010	1.00	2.61
GLU37	HB2	1.00	0.268	0.00	0.00
GLU37	HB3	1.00	0.007	1.00	19.33
GLU37	HG2	1.00	0.003	1.00	2.93
GLU37	HG3	1.00	0.001	1.00	0.67
GLU37	H	1.00	0.005	1.00	-842467.00
LEU38	H	1.00	0.046	0.00	0.00

3.37.8 Detailed Probabilities of GLU37HG2:

Overall probability: 0.859

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU37	1.00	0.86
LEU38	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
E37HA	1.00
E37HB2	1.00
E37HB3	1.00
E37HG3	1.00
E37H	1.00
E37HE2	1.00
E37HG2	1.00
L38H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU37	HA	1.00	0.018	1.00	1.54
GLU37	HB2	1.00	0.001	1.00	0.60
GLU37	HB3	1.00	0.029	1.00	2.85
GLU37	HG2	1.00	0.003	1.00	35.10
GLU37	HG3	1.00	0.002	1.00	4.00
GLU37	H	1.00	0.003	1.00	-484121.00
LEU38	H	0.98	0.313	0.02	0.00

3.37.9 Detailed Probabilities of GLU37HG3:

Overall probability: 0.861

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU37	1.00	0.86
LEU38	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
E37HA	1.00
E37HB2	1.00
E37HB3	1.00
E37HG2	1.00
E37H	1.00
E37HE2	1.00
E37HG3	1.00
L38H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU37	HA	1.00	0.004	1.00	0.36
GLU37	HB2	1.00	0.002	1.00	0.40
GLU37	HB3	1.00	0.001	1.00	0.38
GLU37	HG2	1.00	0.000	1.00	4.17
GLU37	HG3	1.00	0.002	1.00	5.72
GLU37	H	1.00	0.010	1.00	-889219.00
LEU38	H	0.97	0.599	0.03	0.00

3.37.10 Detailed Probabilities of GLU37H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP36	1.00	1.00
GLU37	1.00	1.00
LEU38	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D36H	1.00
D36HA	1.00
D36HB3	1.00
D36HB2	1.00
E37HA	1.00
E37HB2	1.00
E37HB3	1.00
E37HG2	1.00
E37HG3	1.00
E37H	1.00
L38H	1.00

NOESY contacts detailed probability

3.37 GLU(37)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP36	HA	1.00	0.004	1.00	0.20
ASP36	HB2	1.00	0.006	1.00	0.62
ASP36	HB3	1.00	0.003	1.00	0.56
ASP36	H	1.00	0.003	1.00	-1787374.00
GLU37	HA	1.00	0.002	1.00	0.46
GLU37	HB2	1.00	0.004	1.00	0.38
GLU37	HB3	1.00	0.005	1.00	0.41
GLU37	HG2	1.00	0.004	1.00	0.43
GLU37	HG3	1.00	0.004	1.00	0.70
GLU37	H	1.00	0.003	1.00	-6948421.00
LEU38	H	1.00	0.004	1.00	-755753.00
LEU38	HA	0.93	0.008	1.00	0.06

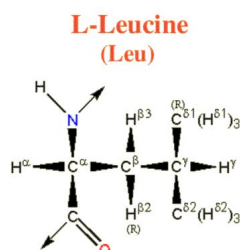
3.38 LEU(38)

Figure 37: Image from the BMRB

Residue probability: 0.614

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	177.649	177.056	1.929	0.000	0.000
CA 3.38.1	59.133	55.735	3.802	0.645	1.000
CB 3.38.2	41.069	42.389	3.750	0.750	1.000
CG 3.38.3	27.177	26.892	3.086	0.500	1.000
CD1 3.38.4	25.761	24.837	3.657	0.686	1.000
CD2 3.38.5	25.562	24.201	3.117	0.657	1.000
N 3.38.6	119.580	121.785	4.943	0.575	1.000
HA 3.38.7	3.911	4.315	0.840	0.600	1.000
HB2 3.38.8	2.114	1.601	0.373	0.850	1.000
HB3 3.38.9	1.461	1.508	0.398	0.556	1.000
HG 3.38.10	1.521	1.510	0.340	0.265	1.000
HD1 3.38.11	0.962	0.739	0.294	0.429	1.000
HD2 3.38.12	0.889	0.727	0.421	0.714	1.000
H 3.38.13	8.203	8.237	0.647	0.757	1.000

3.38.1 Detailed Probabilities of LEU38CA:

Overall probability: 0.645

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU37	0.50	1.00
LEU38	0.73	1.00
LYS39	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E37HA	1.00
L38HB2	1.00
L38HB3	1.00
L38HG	1.00
L38HD11	0.99
L38HD21	0.99
L38H	1.00
L38HA	1.00
K39HA	1.00
K39H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU37	HA	1.00	0.140	0.00	0.00
GLU37	H	0.93	0.008	1.00	0.06
LEU38	HA	1.00	0.008	1.00	5.06
LEU38	HB2	1.00	0.632	0.00	0.00
LEU38	HB3	1.00	0.021	1.00	0.67
LEU38	HG	1.00	0.039	0.10	0.00
LEU38	HD11	0.99	0.001	1.00	0.86
LEU38	HD21	0.99	0.018	1.00	1.38
LEU38	H	1.00	0.011	1.00	0.53
LYS39	HA	1.00	0.078	0.00	0.00
LYS39	H	1.00	0.000	1.00	0.09

3.38.2 Detailed Probabilities of LEU38CB:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU38	0.71	1.00
LYS39	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L38HA	1.00
L38HB3	1.00
L38HG	1.00
L38HD11	1.00
L38HD21	1.00
L38H	1.00
L38HB2	1.00
K39H	1.00

NOESY contacts detailed probability

3.38 LEU(38)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU38	HA	1.00	0.010	1.00	0.29
LEU38	HB2	1.00	0.007	1.00	0.84
LEU38	HB3	1.00	0.013	1.00	0.75
LEU38	HG	1.00	0.047	0.00	0.00
LEU38	HD11	1.00	0.081	0.00	0.00
LEU38	HD21	1.00	0.008	1.00	0.51
LEU38	H	1.00	0.009	1.00	0.36
LYS39	H	1.00	0.004	1.00	0.21

3.38.3 Detailed Probabilities of LEU38CG:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU38	0.43	1.00
LYS39	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L38HA	1.00
L38HB2	1.00
L38HB3	1.00
L38HD11	1.00
L38HD21	1.00
L38H	1.00
L38HG	1.00
K39H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU38	HA	1.00	0.174	0.00	0.00
LEU38	HB2	1.00	0.005	1.00	0.51
LEU38	HB3	1.00	0.515	0.00	0.00
LEU38	HG	1.00	0.455	0.00	0.00
LEU38	HD11	1.00	0.075	0.00	0.00
LEU38	HD21	1.00	0.002	1.00	1.36
LEU38	H	1.00	0.008	1.00	0.16
LYS39	H	0.98	0.006	1.00	0.14

3.38.4 Detailed Probabilities of LEU38CD1:

Overall probability: 0.686

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU38	0.69	1.00

Expected NOESY Contacts

Proton	Expected probability
L38HA	0.99
L38HB2	1.00
L38HB3	1.00
L38HG	1.00
L38HD12	1.00
L38HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU38	HA	0.99	0.011	1.00	1.10
LEU38	HB2	1.00	0.032	0.80	0.00
LEU38	HB3	1.00	0.051	0.00	0.00
LEU38	HG	1.00	0.009	1.00	1.03
LEU38	HD11	1.00	0.003	1.00	42.22
LEU38	HD21	1.00	0.076	0.00	0.00
LEU38	H	0.86	0.008	1.00	0.14

3.38.5 Detailed Probabilities of LEU38CD2:

Overall probability: 0.657

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU38	0.66	1.00

Expected NOESY Contacts

Proton	Expected probability
L38HA	0.99
L38HB2	1.00
L38HB3	1.00
L38HG	1.00
L38HD11	1.00
L38HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU38	HA	0.99	0.034	0.60	0.00
LEU38	HB2	1.00	0.015	1.00	1.09
LEU38	HB3	1.00	0.048	0.00	0.00
LEU38	HG	1.00	0.012	1.00	1.68
LEU38	HD11	1.00	0.486	0.00	0.00
LEU38	HD21	1.00	0.013	1.00	147.68
LEU38	H	0.85	0.005	1.00	0.35

3.38.6 Detailed Probabilities of LEU38N:

Overall probability: 0.575

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU37	0.34	1.00
LEU38	0.71	1.00
LYS39	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E37HB2	1.00
E37HG2	0.98
E37HG3	0.97
E37HB3	1.00
E37H	1.00
E37HA	1.00
L38HA	1.00
L38HB2	1.00
L38HB3	1.00
L38HG	1.00
L38H	1.00
K39H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU37	HA	1.00	0.005	1.00	-580741.00
GLU37	HB2	1.00	0.140	0.00	0.00
GLU37	HB3	1.00	0.046	0.00	0.00
GLU37	HG2	0.98	0.313	0.02	0.00
GLU37	HG3	0.97	0.599	0.03	0.00
GLU37	H	1.00	0.004	1.00	-755753.00
LEU38	HA	1.00	0.003	1.00	-677587.00
LEU38	HB2	1.00	0.015	1.00	-1154493.00
LEU38	HB3	1.00	0.011	1.00	-1002986.00
LEU38	HG	1.00	0.049	0.00	0.00
LEU38	H	1.00	0.179	0.00	0.00
LEU38	HD11	0.88	0.006	1.00	-277297.00
LEU38	HD21	0.87	0.023	1.00	-1213214.00
LYS39	H	1.00	0.008	1.00	-643544.00

3.38.7 Detailed Probabilities of LEU38HA:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU37	0.50	1.00
LEU38	0.66	1.00
LYS39	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E37HA	1.00
L38HB2	1.00
L38HB3	1.00
L38HG	1.00
L38HD11	0.99
L38HD21	0.99
L38H	1.00
L38HA	1.00
K39HA	1.00
K39H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU37	HA	1.00	0.098	0.00	0.00
GLU37	H	0.93	0.015	1.00	-108913.00
LEU38	HA	1.00	0.008	1.00	5.06
LEU38	HB2	1.00	0.010	1.00	0.29
LEU38	HB3	1.00	1.338	0.00	0.00
LEU38	HG	1.00	0.174	0.00	0.00
LEU38	HD11	0.99	0.011	1.00	1.10
LEU38	HD21	0.99	0.034	0.60	0.00
LEU38	H	1.00	0.003	1.00	-677587.00
LYS39	HA	1.00	0.075	0.00	0.00
LYS39	H	1.00	0.026	1.00	-562370.00

3.38.8 Detailed Probabilities of LEU38HB2:

Overall probability: 0.850

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU38	0.83	1.00
LYS39	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L38HA	1.00
L38HB3	1.00
L38HG	1.00
L38HD11	1.00
L38HD21	1.00
L38H	1.00
L38HB2	1.00
K39H	1.00

NOESY contacts detailed probability

3.38 LEU(38)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU38	HA	1.00	0.632	0.00	0.00
LEU38	HB2	1.00	0.007	1.00	0.84
LEU38	HB3	1.00	0.006	1.00	0.67
LEU38	HG	1.00	0.005	1.00	0.51
LEU38	HD11	1.00	0.032	0.80	0.00
LEU38	HD21	1.00	0.015	1.00	1.09
LEU38	H	1.00	0.015	1.00	-1154493.00
LYS39	H	1.00	0.005	1.00	-727324.00

3.38.9 Detailed Probabilities of LEU38HB3:

Overall probability: 0.556

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU38	0.43	1.00
LYS39	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L38HA	1.00
L38HB2	1.00
L38HG	1.00
L38HD11	1.00
L38HD21	1.00
L38H	1.00
L38HB3	1.00
K39H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU38	HA	1.00	0.021	1.00	0.67
LEU38	HB2	1.00	0.013	1.00	0.75
LEU38	HB3	1.00	0.285	0.00	0.00
LEU38	HG	1.00	0.515	0.00	0.00
LEU38	HD11	1.00	0.051	0.00	0.00
LEU38	HD21	1.00	0.048	0.00	0.00
LEU38	H	1.00	0.011	1.00	-1002986.00
LYS39	H	1.00	0.008	1.00	-823304.00
LYS39	HA	0.90	0.022	1.00	1.02

3.38.10 Detailed Probabilities of LEU38HG:

Overall probability: 0.265

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU38	0.30	1.00
LYS39	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
L38HA	1.00
L38HB2	1.00
L38HB3	1.00
L38HD11	1.00
L38HD21	1.00
L38H	1.00
L38HG	1.00
K39H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU38	HA	1.00	0.039	0.10	0.00
LEU38	HB2	1.00	0.047	0.00	0.00
LEU38	HB3	1.00	0.225	0.00	0.00
LEU38	HG	1.00	0.455	0.00	0.00
LEU38	HD11	1.00	0.009	1.00	1.03
LEU38	HD21	1.00	0.012	1.00	1.68
LEU38	H	1.00	0.049	0.00	0.00
LYS39	H	0.98	0.052	0.02	0.00

3.38.11 Detailed Probabilities of LEU38HD11:

Overall probability: 0.429

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU38	0.43	1.00

Expected NOESY Contacts

Proton	Expected probability
L38HA	0.99
L38HB2	1.00
L38HB3	1.00
L38HG	1.00
L38HD12	1.00
L38HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU38	HA	0.99	0.001	1.00	0.86
LEU38	HB2	1.00	0.081	0.00	0.00
LEU38	HB3	1.00	0.784	0.00	0.00
LEU38	HG	1.00	0.075	0.00	0.00
LEU38	HD11	1.00	0.003	1.00	42.22
LEU38	HD21	1.00	0.486	0.00	0.00
LEU38	H	0.86	0.006	1.00	-277297.00

3.38.12 Detailed Probabilities of LEU38HD21:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU38	0.71	1.00

Expected NOESY Contacts

Proton	Expected probability
L38HA	0.99
L38HB2	1.00
L38HB3	1.00
L38HG	1.00
L38HD11	1.00
L38HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU38	HA	0.99	0.018	1.00	1.38
LEU38	HB2	1.00	0.008	1.00	0.51
LEU38	HB3	1.00	0.857	0.00	0.00
LEU38	HG	1.00	0.002	1.00	1.36
LEU38	HD11	1.00	0.076	0.00	0.00
LEU38	HD21	1.00	0.013	1.00	147.68
LEU38	H	0.85	0.023	1.00	-1213214.00

3.38.13 Detailed Probabilities of LEU38H:

Overall probability: 0.757

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU37	0.77	1.00
LEU38	0.71	1.00
LYS39	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E37HB2	1.00
E37HG2	0.98
E37HG3	0.97
E37HB3	1.00
E37H	1.00
E37HA	1.00
L38HA	1.00
L38HB2	1.00
L38HB3	1.00
L38HG	1.00
L38H	1.00
K39H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU37	HA	1.00	0.034	0.60	0.00
GLU37	HB2	1.00	0.010	1.00	0.20
GLU37	HB3	1.00	0.089	0.00	0.00
GLU37	HG2	0.98	0.026	1.00	0.08
GLU37	HG3	0.97	0.008	1.00	0.11
GLU37	H	1.00	0.007	1.00	-760971.00
LEU38	HA	1.00	0.011	1.00	0.53
LEU38	HB2	1.00	0.009	1.00	0.36
LEU38	HB3	1.00	0.149	0.00	0.00
LEU38	HG	1.00	0.008	1.00	0.16
LEU38	H	1.00	0.179	0.00	0.00
LEU38	HD11	0.88	0.008	1.00	0.14
LEU38	HD21	0.87	0.005	1.00	0.35
LYS39	H	1.00	0.004	1.00	-601490.00

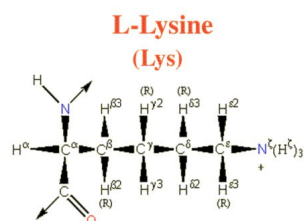


Figure 38: Image from the BMRB

Residue probability: 0.839
Residue probability confidence: 0.945

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	179.577	176.660	3.133	0.000	0.000
CA 3.39.1	59.866	57.014	3.028	0.767	1.000
CB 3.39.2	32.048	32.981	3.186	0.730	1.000
CG 3.39.3	25.419	24.941	1.956	0.913	0.917
CD 3.39.4	29.306	29.020	2.193	0.900	0.900
CE 3.39.5	41.780	41.893	1.492	1.000	0.889
N 3.39.6	118.404	120.954	4.210	0.857	1.000
NZ	NA	—	—	0.000	0.000
HA 3.39.7	3.841	4.262	0.489	0.846	1.000
HB2 3.39.8	1.934	1.774	0.365	0.817	1.000
HB3 3.39.9	1.948	1.742	0.385	0.750	1.000
HG2 3.39.10	1.457	1.358	0.344	0.727	0.917
HG3 3.39.11	1.698	1.343	0.357	0.822	0.917
HD2 3.39.12	1.705	1.614	0.957	0.900	0.900
HD3 3.39.13	1.704	1.595	0.387	0.900	0.900
HE2 3.39.14	2.979	2.907	0.230	0.753	0.889
HE3 3.39.15	2.981	2.901	0.241	0.753	0.889
H 3.39.16	7.829	8.185	0.605	0.988	1.000
HZ	NA	—	—	0.000	0.000

3.39.1 Detailed Probabilities of LYS39CA:

Overall probability: 0.767
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU38	0.50	1.00
LYS39	1.00	1.00
LYS40	0.10	1.00

Expected NOESY Contacts

Proton	Expected probability
L38HA	1.00
K39HB2	1.00
K39HB3	1.00
K39HG2	1.00
K39HG3	1.00
K39HD2	0.98
K39HD3	0.98
K39H	1.00
K39HA	1.00
K40HA	1.00
K40H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU38	HA	1.00	0.075	0.00	0.00
LEU38	HB3	0.90	0.022	1.00	1.02
LYS39	HA	1.00	0.005	1.00	20.35
LYS39	HB2	1.00	0.016	1.00	3.14
LYS39	HB3	1.00	0.030	1.00	0.00
LYS39	HG2	1.00	0.018	1.00	1.02
LYS39	HG3	1.00	0.003	1.00	1.06
LYS39	HD2	0.98	0.004	1.00	1.06
LYS39	HD3	0.98	0.003	1.00	1.06
LYS39	H	1.00	0.012	1.00	0.96
LYS40	HA	1.00	0.089	0.00	0.00
LYS40	H	1.00	0.038	0.20	0.00

3.39.2 Detailed Probabilities of LYS39CB:

Overall probability: 0.730

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS39	0.70	1.00
LYS40	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K39HA	1.00
K39HB3	1.00
K39HG2	1.00
K39HG3	1.00
K39HD2	1.00
K39HD3	1.00
K39HE2	0.98
K39HE3	0.99
K39H	1.00
K39HB2	1.00
K40H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS39	HA	1.00	0.020	1.00	2.44
LYS39	HB2	1.00	0.030	1.00	0.00
LYS39	HB3	1.00	0.241	0.00	0.00
LYS39	HG2	1.00	0.016	1.00	3.41
LYS39	HG3	1.00	0.015	1.00	5.56
LYS39	HD2	1.00	0.022	1.00	5.56
LYS39	HD3	1.00	0.021	1.00	5.56
LYS39	HE2	0.98	0.050	0.02	0.00
LYS39	HE3	0.99	0.052	0.01	0.00
LYS39	H	1.00	0.022	1.00	2.95
LYS40	H	1.00	0.028	1.00	2.95

3.39.3 Detailed Probabilities of LYS39CG:

Overall probability: 0.913

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS39	1.00	0.91
LYS40	0.04	1.00

Expected NOESY Contacts

Proton	Expected probability
K39HA	1.00
K39HB2	1.00
K39HB3	1.00
K39HG2	1.00
K39HD2	1.00
K39HD3	1.00
K39HE2	1.00
K39HE3	1.00
K39H	1.00
K39HZ2	1.00
K39HG3	1.00
K40H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS39	HA	1.00	0.000	1.00	0.36
LYS39	HB2	1.00	0.004	1.00	1.27
LYS39	HB3	1.00	0.010	1.00	1.27
LYS39	HG2	1.00	0.003	1.00	3.47
LYS39	HG3	1.00	0.011	1.00	11.48
LYS39	HD2	1.00	0.004	1.00	11.48
LYS39	HD3	1.00	0.005	1.00	11.48
LYS39	HE2	1.00	0.029	1.00	0.55
LYS39	HE3	1.00	0.027	1.00	0.55
LYS39	H	1.00	0.003	1.00	0.45
LYS40	H	0.96	0.047	0.04	0.00

3.39.4 Detailed Probabilities of LYS39CD:

Overall probability: 0.900

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS39	0.90	0.90

Expected NOESY Contacts

Proton	Expected probability
K39HA	0.98
K39HB2	1.00
K39HB3	1.00
K39HG2	1.00
K39HG3	1.00
K39HD3	1.00
K39HE2	1.00
K39HE3	1.00
K39HZ2	1.00
K39HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS39	HA	0.98	0.002	1.00	0.37
LYS39	HB2	1.00	0.002	1.00	5.45
LYS39	HB3	1.00	0.016	1.00	5.45
LYS39	HG2	1.00	0.054	0.00	0.00
LYS39	HG3	1.00	0.014	1.00	244.35
LYS39	HD2	1.00	0.021	1.00	244.35
LYS39	HD3	1.00	0.020	1.00	244.35
LYS39	HE2	1.00	0.003	1.00	6.07
LYS39	HE3	1.00	0.001	1.00	6.07
LYS39	H	0.88	0.020	1.00	0.52

3.39.5 Detailed Probabilities of LYS39CE:

Overall probability: 1.000

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS39	1.00	0.89

Expected NOESY Contacts

Proton	Expected probability
K39HB2	0.98
K39HB3	0.99
K39HG2	1.00
K39HG3	1.00
K39HD2	1.00
K39HD3	1.00
K39HE3	1.00
K39HZ2	1.00
K39HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS39	HB2	0.98	0.004	1.00	1.41
LYS39	HB3	0.99	0.018	1.00	1.41
LYS39	HG2	1.00	0.008	1.00	1.66
LYS39	HG3	1.00	0.002	1.00	15.02
LYS39	HD2	1.00	0.009	1.00	15.02
LYS39	HD3	1.00	0.008	1.00	15.02
LYS39	HE2	1.00	0.008	1.00	641.65
LYS39	HE3	1.00	0.006	1.00	641.65
LYS39	HA	0.77	0.001	1.00	0.07

3.39.6 Detailed Probabilities of LYS39N:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU38	0.84	1.00
LYS39	0.96	1.00
LYS40	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
L38HA	1.00
L38H	1.00
L38HB3	1.00
L38HB2	1.00
L38HG	0.98
K39HA	1.00
K39HB2	1.00
K39HB3	1.00
K39HG2	1.00
K39HG3	1.00
K39H	1.00
K40H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU38	HA	1.00	0.026	1.00	-562370.00
LEU38	HB2	1.00	0.005	1.00	-727324.00
LEU38	HB3	1.00	0.008	1.00	-823304.00
LEU38	HG	0.98	0.052	0.02	0.00
LEU38	H	1.00	0.004	1.00	-601490.00
LEU38	HD21	0.59	0.019	1.00	-738227.00
LYS39	HA	1.00	0.001	1.00	-913966.00
LYS39	HB2	1.00	0.033	0.70	0.00
LYS39	HB3	1.00	0.019	1.00	-1741079.00
LYS39	HG2	1.00	0.012	1.00	-823304.00
LYS39	HG3	1.00	0.004	1.00	-1065772.00
LYS39	H	1.00	0.003	1.00	-12164598.00
LYS39	HD2	0.88	0.003	1.00	-1065772.00
LYS39	HD3	0.87	0.002	1.00	-1065772.00
LYS40	H	1.00	0.047	0.00	0.00
LYS40	HB2	0.61	0.023	1.00	-1741079.00

3.39.7 Detailed Probabilities of LYS39HA:

Overall probability: 0.846

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU38	0.00	1.00
LYS39	1.00	1.00
LYS40	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
L38HA	1.00
K39HB2	1.00
K39HB3	1.00
K39HG2	1.00
K39HG3	1.00
K39HD2	0.98
K39HD3	0.98
K39H	1.00
K39HA	1.00
K40HA	1.00
K40H	1.00

NOESY contacts detailed probability

3.39 LYS(39)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU38	HA	1.00	0.078	0.00	0.00
LYS39	HA	1.00	0.005	1.00	20.35
LYS39	HB2	1.00	0.020	1.00	2.44
LYS39	HB3	1.00	0.020	1.00	2.44
LYS39	HG2	1.00	0.000	1.00	0.55
LYS39	HG3	1.00	0.000	1.00	0.36
LYS39	HD2	0.98	0.002	1.00	0.37
LYS39	HD3	0.98	0.002	1.00	0.37
LYS39	H	1.00	0.001	1.00	-913966.00
LYS39	HE2	0.77	0.001	1.00	0.07
LYS39	HE3	0.76	0.001	1.00	0.07
LYS40	HA	1.00	0.201	0.00	0.00
LYS40	H	1.00	0.021	1.00	-359301.00

3.39.8 Detailed Probabilities of LYS39HB2:

Overall probability: 0.817

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS39	0.87	1.00
LYS40	0.55	1.00

Expected NOESY Contacts

Proton	Expected probability
K39HA	1.00
K39HB3	1.00
K39HG2	1.00
K39HG3	1.00
K39HD2	1.00
K39HD3	1.00
K39HE2	0.98
K39HE3	0.99
K39H	1.00
K39HB2	1.00
K40H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS39	HA	1.00	0.016	1.00	3.14
LYS39	HB2	1.00	0.030	1.00	0.00
LYS39	HB3	1.00	0.030	1.00	0.00
LYS39	HG2	1.00	0.069	0.00	0.00
LYS39	HG3	1.00	0.004	1.00	1.27
LYS39	HD2	1.00	0.002	1.00	5.45
LYS39	HD3	1.00	0.002	1.00	5.45
LYS39	HE2	0.98	0.004	1.00	1.41
LYS39	HE3	0.99	0.004	1.00	1.41
LYS39	H	1.00	0.033	0.70	0.00
LYS40	H	1.00	0.039	0.10	0.00
LYS40	HA	0.64	0.007	1.00	3.48

3.39.9 Detailed Probabilities of LYS39HB3:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS39	0.70	1.00
LYS40	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K39HA	1.00
K39HB2	1.00
K39HG2	1.00
K39HG3	1.00
K39HD2	1.00
K39HD3	1.00
K39HE2	0.99
K39HE3	0.99
K39H	1.00
K39HB3	1.00
K40H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS39	HA	1.00	0.030	1.00	0.00
LYS39	HB2	1.00	0.241	0.00	0.00
LYS39	HB3	1.00	0.241	0.00	0.00
LYS39	HG2	1.00	0.055	0.00	0.00
LYS39	HG3	1.00	0.010	1.00	1.27
LYS39	HD2	1.00	0.016	1.00	5.45
LYS39	HD3	1.00	0.016	1.00	5.45
LYS39	HE2	0.99	0.018	1.00	1.41
LYS39	HE3	0.99	0.018	1.00	1.41
LYS39	H	1.00	0.019	1.00	-1741079.00
LYS40	H	1.00	0.025	1.00	-3345797.00
LYS40	HA	0.82	0.007	1.00	3.48

3.39.10 Detailed Probabilities of LYS39HG2:

Overall probability: 0.727

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS39	0.70	0.91
LYS40	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K39HA	1.00
K39HB2	1.00
K39HB3	1.00
K39HG3	1.00
K39HD2	1.00
K39HD3	1.00
K39HE2	1.00
K39HE3	1.00
K39H	1.00
K39HZ2	1.00
K39HG2	1.00
K40H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS39	HA	1.00	0.018	1.00	1.02
LYS39	HB2	1.00	0.016	1.00	3.41
LYS39	HB3	1.00	0.016	1.00	3.41
LYS39	HG2	1.00	0.115	0.00	0.00
LYS39	HG3	1.00	0.003	1.00	3.47
LYS39	HD2	1.00	0.054	0.00	0.00
LYS39	HD3	1.00	0.054	0.00	0.00
LYS39	HE2	1.00	0.008	1.00	1.66
LYS39	HE3	1.00	0.008	1.00	1.66
LYS39	H	1.00	0.012	1.00	-823304.00
LYS40	H	0.97	0.024	1.00	-519075.00

3.39.11 Detailed Probabilities of LYS39HG3:

Overall probability: 0.822

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS39	0.90	0.91
LYS40	0.04	1.00

Expected NOESY Contacts

Proton	Expected probability
K39HA	1.00
K39HB2	1.00
K39HB3	1.00
K39HG2	1.00
K39HD2	1.00
K39HD3	1.00
K39HE2	1.00
K39HE3	1.00
K39H	1.00
K39HZ2	1.00
K39HG3	1.00
K40H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS39	HA	1.00	0.003	1.00	1.06
LYS39	HB2	1.00	0.015	1.00	5.56
LYS39	HB3	1.00	0.015	1.00	5.56
LYS39	HG2	1.00	0.094	0.00	0.00
LYS39	HG3	1.00	0.011	1.00	11.48
LYS39	HD2	1.00	0.014	1.00	244.35
LYS39	HD3	1.00	0.014	1.00	244.35
LYS39	HE2	1.00	0.002	1.00	15.02
LYS39	HE3	1.00	0.002	1.00	15.02
LYS39	H	1.00	0.004	1.00	-1065772.00
LYS40	H	0.96	0.062	0.04	0.00

3.39.12 Detailed Probabilities of LYS39HD2:

Overall probability: 0.900

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS39	0.90	0.90

Expected NOESY Contacts

Proton	Expected probability
K39HA	0.98
K39HB2	1.00
K39HB3	1.00
K39HG2	1.00
K39HG3	1.00
K39HD3	1.00
K39HE2	1.00
K39HE3	1.00
K39HZ2	1.00
K39HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS39	HA	0.98	0.004	1.00	1.06
LYS39	HB2	1.00	0.022	1.00	5.56
LYS39	HB3	1.00	0.022	1.00	5.56
LYS39	HG2	1.00	0.101	0.00	0.00
LYS39	HG3	1.00	0.004	1.00	11.48
LYS39	HD2	1.00	0.021	1.00	244.35
LYS39	HD3	1.00	0.021	1.00	244.35
LYS39	HE2	1.00	0.009	1.00	15.02
LYS39	HE3	1.00	0.009	1.00	15.02
LYS39	H	0.88	0.003	1.00	-1065772.00

3.39.13 Detailed Probabilities of LYS39HD3:

Overall probability: 0.900

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS39	0.90	0.90

Expected NOESY Contacts

Proton	Expected probability
K39HA	0.98
K39HB2	1.00
K39HB3	1.00
K39HG2	1.00
K39HG3	1.00
K39HD2	1.00
K39HE2	1.00
K39HE3	1.00
K39HZ2	1.00
K39HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS39	HA	0.98	0.003	1.00	1.06
LYS39	HB2	1.00	0.021	1.00	5.56
LYS39	HB3	1.00	0.021	1.00	5.56
LYS39	HG2	1.00	0.100	0.00	0.00
LYS39	HG3	1.00	0.005	1.00	11.48
LYS39	HD2	1.00	0.020	1.00	244.35
LYS39	HD3	1.00	0.020	1.00	244.35
LYS39	HE2	1.00	0.008	1.00	15.02
LYS39	HE3	1.00	0.008	1.00	15.02
LYS39	H	0.87	0.002	1.00	-1065772.00

3.39.14 Detailed Probabilities of LYS39HE2:

Overall probability: 0.753

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS39	0.75	0.89

Expected NOESY Contacts

Proton	Expected probability
K39HB2	0.98
K39HB3	0.99
K39HG2	1.00
K39HG3	1.00
K39HD2	1.00
K39HD3	1.00
K39HE3	1.00
K39HZ2	1.00
K39HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS39	HB2	0.98	0.050	0.02	0.00
LYS39	HB3	0.99	0.050	0.01	0.00
LYS39	HG2	1.00	0.019	1.00	0.86
LYS39	HG3	1.00	0.029	1.00	0.55
LYS39	HD2	1.00	0.003	1.00	6.07
LYS39	HD3	1.00	0.003	1.00	6.07
LYS39	HE2	1.00	0.008	1.00	641.65
LYS39	HE3	1.00	0.008	1.00	641.65

3.39.15 Detailed Probabilities of LYS39HE3:

Overall probability: 0.753

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS39	0.75	0.89

Expected NOESY Contacts

Proton	Expected probability
K39HB2	0.99
K39HB3	0.99
K39HG2	1.00
K39HG3	1.00
K39HD2	1.00
K39HD3	1.00
K39HE2	1.00
K39HZ2	1.00
K39HE3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS39	HB2	0.99	0.052	0.01	0.00
LYS39	HB3	0.99	0.052	0.01	0.00
LYS39	HG2	1.00	0.021	1.00	0.86
LYS39	HG3	1.00	0.027	1.00	0.55
LYS39	HD2	1.00	0.001	1.00	6.07
LYS39	HD3	1.00	0.001	1.00	6.07
LYS39	HE2	1.00	0.006	1.00	641.65
LYS39	HE3	1.00	0.006	1.00	641.65

3.39.16 Detailed Probabilities of LYS39H:

Overall probability: 0.988

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU38	1.00	1.00
LYS39	1.00	1.00
LYS40	0.90	1.00

Expected NOESY Contacts

Proton	Expected probability
L38HA	1.00
L38H	1.00
L38HB3	1.00
L38HB2	1.00
L38HG	0.98
K39HA	1.00
K39HB2	1.00
K39HB3	1.00
K39HG2	1.00
K39HG3	1.00
K39H	1.00
K40H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU38	HA	1.00	0.000	1.00	0.09
LEU38	HB2	1.00	0.004	1.00	0.21
LEU38	HB3	1.00	0.001	1.00	0.17
LEU38	HG	0.98	0.006	1.00	0.14
LEU38	H	1.00	0.008	1.00	-643544.00
LEU38	HD11	0.52	0.010	1.00	0.17
LEU38	HD21	0.59	0.011	1.00	0.36
LYS39	HA	1.00	0.012	1.00	0.96
LYS39	HB2	1.00	0.022	1.00	2.95
LYS39	HB3	1.00	0.022	1.00	2.95
LYS39	HG2	1.00	0.020	1.00	0.45
LYS39	HG3	1.00	0.003	1.00	0.45
LYS39	H	1.00	0.003	1.00	-12164598.00
LYS39	HD2	0.88	0.020	1.00	0.52
LYS39	HD3	0.87	0.020	1.00	0.52
LYS40	H	1.00	0.032	0.80	0.00
LYS40	HB2	0.61	0.022	1.00	2.95

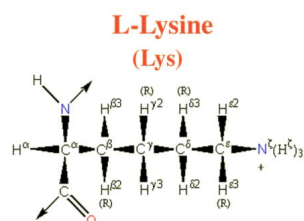


Figure 39: Image from the BMRB

Residue probability: 0.674
Residue probability confidence: 0.945

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	179.577	176.660	3.133	0.000	0.000
CA 3.40.1	59.590	57.014	3.028	0.692	1.000
CB 3.40.2	32.400	32.981	3.186	0.336	1.000
CG 3.40.3	24.982	24.941	1.956	0.727	0.917
CD 3.40.4	29.333	29.020	2.193	0.800	0.900
CE 3.40.5	41.780	41.893	1.492	0.839	0.889
N 3.40.6	119.271	120.954	4.210	0.796	1.000
NZ	NA	—	—	0.000	0.000
HA 3.40.7	4.022	4.262	0.489	0.636	1.000
HB2 3.40.8	1.990	1.774	0.365	0.112	1.000
HB3 3.40.9	1.945	1.742	0.385	0.833	1.000
HG2 3.40.10	1.379	1.358	0.344	0.818	0.917
HG3 3.40.11	1.620	1.343	0.357	0.473	0.917
HD2 3.40.12	1.681	1.614	0.957	0.667	0.900
HD3 3.40.13	1.680	1.595	0.387	0.667	0.900
HE2 3.40.14	2.968	2.907	0.230	0.764	0.889
HE3 3.40.15	2.966	2.901	0.241	0.789	0.889
H 3.40.16	7.779	8.185	0.605	0.828	1.000
HZ	NA	—	—	0.000	0.000

3.40.1 Detailed Probabilities of LYS40CA:

Overall probability: 0.692
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS39	0.67	1.00
LYS40	0.75	1.00
GLU41	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K39HA	1.00
K40HB2	1.00
K40HB3	1.00
K40HG2	1.00
K40HG3	1.00
K40HD2	0.98
K40HD3	0.98
K40H	1.00
K40HA	1.00
E41HA	1.00
E41H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS39	HA	1.00	0.201	0.00	0.00
LYS39	HB2	0.64	0.007	1.00	3.48
LYS39	HB3	0.82	0.007	1.00	3.48
LYS40	HA	1.00	0.020	1.00	41.95
LYS40	HB2	1.00	0.049	0.00	0.00
LYS40	HB3	1.00	0.004	1.00	3.48
LYS40	HG2	1.00	0.025	1.00	1.34
LYS40	HG3	1.00	0.081	0.00	0.00
LYS40	HD2	0.98	0.020	1.00	1.39
LYS40	HD3	0.98	0.021	1.00	1.39
LYS40	H	1.00	0.014	1.00	1.15
GLU41	HA	1.00	0.221	0.00	0.00
GLU41	H	1.00	0.015	1.00	0.28

3.40.2 Detailed Probabilities of LYS40CB:

Overall probability: 0.336

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS40	0.37	1.00
GLU41	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K40HA	1.00
K40HB2	1.00
K40HG2	1.00
K40HG3	1.00
K40HD2	1.00
K40HD3	1.00
K40HE2	0.99
K40HE3	0.99
K40H	1.00
K40HB3	1.00
E41H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS40	HA	1.00	0.201	0.00	0.00
LYS40	HB2	1.00	0.199	0.00	0.00
LYS40	HB3	1.00	0.244	0.00	0.00
LYS40	HG2	1.00	0.204	0.00	0.00
LYS40	HG3	1.00	0.037	0.30	0.00
LYS40	HD2	1.00	0.002	1.00	5.56
LYS40	HD3	1.00	0.003	1.00	5.56
LYS40	HE2	0.99	0.039	0.10	0.00
LYS40	HE3	0.99	0.037	0.30	0.00
LYS40	H	1.00	0.028	1.00	2.95
GLU41	H	1.00	0.184	0.00	0.00

3.40.3 Detailed Probabilities of LYS40CG:

Overall probability: 0.727

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS40	0.70	0.91
GLU41	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K40HA	1.00
K40HB2	1.00
K40HB3	1.00
K40HG2	1.00
K40HD2	1.00
K40HD3	1.00
K40HE2	1.00
K40HE3	1.00
K40H	1.00
K40HZ2	1.00
K40HG3	1.00
E41H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS40	HA	1.00	0.007	1.00	0.66
LYS40	HB2	1.00	0.146	0.00	0.00
LYS40	HB3	1.00	0.027	1.00	2.64
LYS40	HG2	1.00	0.009	1.00	7.08
LYS40	HG3	1.00	0.005	1.00	25.64
LYS40	HD2	1.00	0.056	0.00	0.00
LYS40	HD3	1.00	0.055	0.00	0.00
LYS40	HE2	1.00	0.003	1.00	0.89
LYS40	HE3	1.00	0.005	1.00	0.89
LYS40	H	1.00	0.008	1.00	0.56
GLU41	H	0.97	0.014	1.00	0.07

3.40.4 Detailed Probabilities of LYS40CD:

Overall probability: 0.800

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS40	0.80	0.90

Expected NOESY Contacts

Proton	Expected probability
K40HA	0.98
K40HB2	1.00
K40HB3	1.00
K40HG2	1.00
K40HG3	1.00
K40HD2	1.00
K40HE2	1.00
K40HE3	1.00
K40HZ2	1.00
K40HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS40	HA	0.98	0.026	1.00	1.33
LYS40	HB2	1.00	0.058	0.00	0.00
LYS40	HB3	1.00	0.013	1.00	5.45
LYS40	HG2	1.00	0.024	1.00	6.19
LYS40	HG3	1.00	0.217	0.00	0.00
LYS40	HD2	1.00	0.003	1.00	244.35
LYS40	HD3	1.00	0.004	1.00	244.35
LYS40	HE2	1.00	0.014	1.00	6.07
LYS40	HE3	1.00	0.016	1.00	6.07
LYS40	H	0.87	0.030	1.00	0.00

3.40.5 Detailed Probabilities of LYS40CE:

Overall probability: 0.839

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS40	0.84	0.89

Expected NOESY Contacts

Proton	Expected probability
K40HB2	0.98
K40HB3	0.99
K40HG2	1.00
K40HG3	1.00
K40HD2	1.00
K40HD3	1.00
K40HE3	1.00
K40HZ2	1.00
K40HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS40	HB2	0.98	0.060	0.02	0.00
LYS40	HB3	0.99	0.015	1.00	1.41
LYS40	HG2	1.00	0.020	1.00	2.36
LYS40	HG3	1.00	0.033	0.70	0.00
LYS40	HD2	1.00	0.015	1.00	15.02
LYS40	HD3	1.00	0.016	1.00	15.02
LYS40	HE2	1.00	0.019	1.00	641.65
LYS40	HE3	1.00	0.021	1.00	641.65

3.40.6 Detailed Probabilities of LYS40N:

Overall probability: 0.796

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS39	0.66	1.00
LYS40	0.83	1.00
GLU41	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K39HB2	1.00
K39HG3	0.96
K39HB3	1.00
K39HA	1.00
K39HG2	0.97
K39H	1.00
K40HA	1.00
K40HB2	1.00
K40HB3	1.00
K40HG2	1.00
K40HG3	1.00
K40H	1.00
E41H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS39	HA	1.00	0.021	1.00	-359301.00
LYS39	HB2	1.00	0.039	0.10	0.00
LYS39	HB3	1.00	0.025	1.00	-3345797.00
LYS39	HG2	0.97	0.024	1.00	-519075.00
LYS39	HG3	0.96	0.062	0.04	0.00
LYS39	H	1.00	0.032	0.80	0.00
LYS40	HA	1.00	0.050	0.00	0.00
LYS40	HB2	1.00	0.017	1.00	-3345797.00
LYS40	HB3	1.00	0.028	1.00	-3345797.00
LYS40	HG2	1.00	0.016	1.00	-397162.00
LYS40	HG3	1.00	0.016	1.00	-959776.00
LYS40	H	1.00	0.018	1.00	-17394328.00
GLU41	H	1.00	0.007	1.00	-980247.00
GLU41	HA	0.87	0.012	1.00	-98765.00
GLU41	HB2	0.66	0.023	1.00	-3345797.00

3.40.7 Detailed Probabilities of LYS40HA:

Overall probability: 0.636

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS39	0.00	1.00
LYS40	0.63	1.00
GLU41	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K39HA	1.00
K40HB2	1.00
K40HB3	1.00
K40HG2	1.00
K40HG3	1.00
K40HD2	0.98
K40HD3	0.98
K40H	1.00
K40HA	1.00
E41HA	1.00
E41H	1.00

NOESY contacts detailed probability

3.40 LYS(40)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS39	HA	1.00	0.089	0.00	0.00
LYS40	HA	1.00	0.020	1.00	41.95
LYS40	HB2	1.00	0.418	0.00	0.00
LYS40	HB3	1.00	0.201	0.00	0.00
LYS40	HG2	1.00	0.015	1.00	0.96
LYS40	HG3	1.00	0.007	1.00	0.66
LYS40	HD2	0.98	0.026	1.00	1.33
LYS40	HD3	0.98	0.026	1.00	1.33
LYS40	H	1.00	0.050	0.00	0.00
GLU41	HA	1.00	0.016	1.00	0.10
GLU41	H	1.00	0.010	1.00	-287422.00

3.40.8 Detailed Probabilities of LYS40HB2:

Overall probability: 0.112

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS40	0.10	1.00
GLU41	0.20	1.00

Expected NOESY Contacts

Proton	Expected probability
K40HA	1.00
K40HB3	1.00
K40HG2	1.00
K40HG3	1.00
K40HD2	1.00
K40HD3	1.00
K40HE2	0.98
K40HE3	0.99
K40H	1.00
K40HB2	1.00
E41H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS40	HA	1.00	0.049	0.00	0.00
LYS40	HB2	1.00	0.986	0.00	0.00
LYS40	HB3	1.00	0.199	0.00	0.00
LYS40	HG2	1.00	0.052	0.00	0.00
LYS40	HG3	1.00	0.146	0.00	0.00
LYS40	HD2	1.00	0.058	0.00	0.00
LYS40	HD3	1.00	0.058	0.00	0.00
LYS40	HE2	0.98	0.060	0.02	0.00
LYS40	HE3	0.99	0.060	0.01	0.00
LYS40	H	1.00	0.017	1.00	-3345797.00
GLU41	H	1.00	0.038	0.20	0.00

3.40.9 Detailed Probabilities of LYS40HB3:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS40	0.80	1.00
GLU41	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K40HA	1.00
K40HB2	1.00
K40HG2	1.00
K40HG3	1.00
K40HD2	1.00
K40HD3	1.00
K40HE2	0.99
K40HE3	0.99
K40H	1.00
K40HB3	1.00
E41H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS40	HA	1.00	0.004	1.00	3.48
LYS40	HB2	1.00	0.941	0.00	0.00
LYS40	HB3	1.00	0.244	0.00	0.00
LYS40	HG2	1.00	0.007	1.00	2.40
LYS40	HG3	1.00	0.027	1.00	2.64
LYS40	HD2	1.00	0.013	1.00	5.45
LYS40	HD3	1.00	0.013	1.00	5.45
LYS40	HE2	0.99	0.015	1.00	1.41
LYS40	HE3	0.99	0.015	1.00	1.41
LYS40	H	1.00	0.028	1.00	-3345797.00
GLU41	H	1.00	0.007	1.00	-1920456.00
GLU41	HA	0.80	0.026	1.00	2.01

3.40.10 Detailed Probabilities of LYS40HG2:

Overall probability: 0.818

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS40	0.80	0.91
GLU41	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K40HA	1.00
K40HB2	1.00
K40HB3	1.00
K40HG3	1.00
K40HD2	1.00
K40HD3	1.00
K40HE2	1.00
K40HE3	1.00
K40H	1.00
K40HZ2	1.00
K40HG2	1.00
E41H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS40	HA	1.00	0.025	1.00	1.34
LYS40	HB2	1.00	0.375	0.00	0.00
LYS40	HB3	1.00	0.204	0.00	0.00
LYS40	HG2	1.00	0.005	1.00	36.93
LYS40	HG3	1.00	0.009	1.00	7.08
LYS40	HD2	1.00	0.024	1.00	6.19
LYS40	HD3	1.00	0.024	1.00	6.19
LYS40	HE2	1.00	0.020	1.00	2.36
LYS40	HE3	1.00	0.020	1.00	2.36
LYS40	H	1.00	0.016	1.00	-397162.00
GLU41	H	0.98	0.024	1.00	-132344.00

3.40.11 Detailed Probabilities of LYS40HG3:

Overall probability: 0.473

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS40	0.47	0.91
GLU41	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K40HA	1.00
K40HB2	1.00
K40HB3	1.00
K40HG2	1.00
K40HD2	1.00
K40HD3	1.00
K40HE2	1.00
K40HE3	1.00
K40H	1.00
K40HZ2	1.00
K40HG3	1.00
E41H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS40	HA	1.00	0.081	0.00	0.00
LYS40	HB2	1.00	0.616	0.00	0.00
LYS40	HB3	1.00	0.037	0.30	0.00
LYS40	HG2	1.00	0.015	1.00	9.44
LYS40	HG3	1.00	0.005	1.00	25.64
LYS40	HD2	1.00	0.217	0.00	0.00
LYS40	HD3	1.00	0.217	0.00	0.00
LYS40	HE2	1.00	0.033	0.70	0.00
LYS40	HE3	1.00	0.033	0.70	0.00
LYS40	H	1.00	0.016	1.00	-959776.00
GLU41	H	0.97	0.035	0.50	0.00

3.40.12 Detailed Probabilities of LYS40HD2:

Overall probability: 0.667

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS40	0.67	0.90

Expected NOESY Contacts

Proton	Expected probability
K40HA	0.98
K40HB2	1.00
K40HB3	1.00
K40HG2	1.00
K40HG3	1.00
K40HD3	1.00
K40HE2	1.00
K40HE3	1.00
K40HZ2	1.00
K40HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS40	HA	0.98	0.020	1.00	1.39
LYS40	HB2	1.00	0.677	0.00	0.00
LYS40	HB3	1.00	0.002	1.00	5.56
LYS40	HG2	1.00	0.046	0.00	0.00
LYS40	HG3	1.00	0.056	0.00	0.00
LYS40	HD2	1.00	0.003	1.00	244.35
LYS40	HD3	1.00	0.003	1.00	244.35
LYS40	HE2	1.00	0.015	1.00	15.02
LYS40	HE3	1.00	0.015	1.00	15.02

3.40.13 Detailed Probabilities of LYS40HD3:

Overall probability: 0.667

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS40	0.67	0.90

Expected NOESY Contacts

Proton	Expected probability
K40HA	0.98
K40HB2	1.00
K40HB3	1.00
K40HG2	1.00
K40HG3	1.00
K40HD2	1.00
K40HE2	1.00
K40HE3	1.00
K40HZ2	1.00
K40HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS40	HA	0.98	0.021	1.00	1.39
LYS40	HB2	1.00	0.676	0.00	0.00
LYS40	HB3	1.00	0.003	1.00	5.56
LYS40	HG2	1.00	0.045	0.00	0.00
LYS40	HG3	1.00	0.055	0.00	0.00
LYS40	HD2	1.00	0.004	1.00	244.35
LYS40	HD3	1.00	0.004	1.00	244.35
LYS40	HE2	1.00	0.016	1.00	15.02
LYS40	HE3	1.00	0.016	1.00	15.02

3.40.14 Detailed Probabilities of LYS40HE2:

Overall probability: 0.764

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS40	0.76	0.89

Expected NOESY Contacts

Proton	Expected probability
K40HB2	0.98
K40HB3	0.99
K40HG2	1.00
K40HG3	1.00
K40HD2	1.00
K40HD3	1.00
K40HE3	1.00
K40HZ2	1.00
K40HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS40	HB2	0.98	0.636	0.02	0.00
LYS40	HB3	0.99	0.039	0.10	0.00
LYS40	HG2	1.00	0.006	1.00	1.13
LYS40	HG3	1.00	0.003	1.00	0.89
LYS40	HD2	1.00	0.014	1.00	6.07
LYS40	HD3	1.00	0.014	1.00	6.07
LYS40	HE2	1.00	0.019	1.00	641.65
LYS40	HE3	1.00	0.019	1.00	641.65

3.40.15 Detailed Probabilities of LYS40HE3:

Overall probability: 0.789

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS40	0.79	0.89

Expected NOESY Contacts

Proton	Expected probability
K40HB2	0.99
K40HB3	0.99
K40HG2	1.00
K40HG3	1.00
K40HD2	1.00
K40HD3	1.00
K40HE2	1.00
K40HZ2	1.00
K40HE3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS40	HB2	0.99	0.638	0.01	0.00
LYS40	HB3	0.99	0.037	0.30	0.00
LYS40	HG2	1.00	0.008	1.00	1.13
LYS40	HG3	1.00	0.005	1.00	0.89
LYS40	HD2	1.00	0.016	1.00	6.07
LYS40	HD3	1.00	0.016	1.00	6.07
LYS40	HE2	1.00	0.021	1.00	641.65
LYS40	HE3	1.00	0.021	1.00	641.65

3.40.16 Detailed Probabilities of LYS40H:

Overall probability: 0.828

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS39	0.66	1.00
LYS40	1.00	1.00
GLU41	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K39HB2	1.00
K39HG3	0.96
K39HB3	1.00
K39HA	1.00
K39HG2	0.97
K39H	1.00
K40HA	1.00
K40HB2	1.00
K40HB3	1.00
K40HG2	1.00
K40HG3	1.00
K40H	1.00
E41H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS39	HA	1.00	0.038	0.20	0.00
LYS39	HB2	1.00	0.028	1.00	2.95
LYS39	HB3	1.00	0.028	1.00	2.95
LYS39	HG2	0.97	0.030	1.00	0.00
LYS39	HG3	0.96	0.047	0.04	0.00
LYS39	H	1.00	0.047	0.00	0.00
LYS39	HD2	0.56	0.030	1.00	0.00
LYS39	HD3	0.59	0.030	1.00	0.00
LYS40	HA	1.00	0.014	1.00	1.15
LYS40	HB2	1.00	0.028	1.00	2.95
LYS40	HB3	1.00	0.028	1.00	2.95
LYS40	HG2	1.00	0.013	1.00	0.36
LYS40	HG3	1.00	0.008	1.00	0.56
LYS40	H	1.00	0.018	1.00	-17394328.00
GLU41	H	1.00	0.007	1.00	-1015424.00
GLU41	HB2	0.66	0.002	1.00	0.06

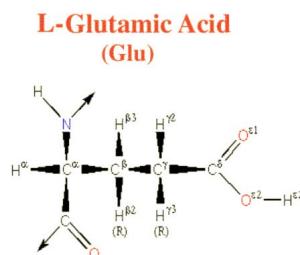


Figure 40: Image from the BMRB

Residue probability: 0.800
Residue probability confidence: 0.925

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	179.504	176.942	2.547	0.000	0.000
CA 3.41.1	58.074	57.442	3.837	0.790	1.000
CB 3.41.2	28.246	30.185	4.018	0.714	0.875
CG 3.41.3	34.904	36.085	1.533	0.860	0.875
N 3.41.4	119.647	120.574	4.837	0.847	1.000
HA 3.41.5	4.263	4.245	0.429	0.700	1.000
HB2 3.41.6	1.950	2.021	0.233	1.000	0.875
HB3 3.41.7	1.949	1.994	0.244	1.000	0.875
HG2 3.41.8	2.133	2.258	0.226	0.431	0.875
HG3 3.41.9	2.459	2.233	0.232	0.857	0.875
H 3.41.10	8.721	8.332	0.601	0.800	1.000
HE2	NA	—	—	0.000	0.000

3.41.1 Detailed Probabilities of GLU41CA:

Overall probability: 0.790
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS40	1.00	1.00
GLU41	0.98	1.00
MET42	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K40HA	1.00
E41HB2	1.00
E41HB3	1.00
E41HG2	1.00
E41HG3	1.00
E41H	1.00
E41HA	1.00
M42HA	1.00
M42H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS40	HA	1.00	0.016	1.00	0.10
LYS40	HB3	0.80	0.026	1.00	2.01
GLU41	HA	1.00	0.019	1.00	12.17
GLU41	HB2	1.00	0.031	0.90	0.00
GLU41	HB3	1.00	0.030	1.00	0.00
GLU41	HG2	1.00	0.015	1.00	0.32
GLU41	HG3	1.00	0.009	1.00	0.20
GLU41	H	1.00	0.011	1.00	0.43
MET42	HA	1.00	0.101	0.00	0.00
MET42	H	1.00	0.047	0.00	0.00

3.41.2 Detailed Probabilities of GLU41CB:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU41	0.83	0.86
MET42	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E41HA	1.00
E41HB3	1.00
E41HG2	1.00
E41HG3	1.00
E41H	1.00
E41HE2	1.00
E41HB2	1.00
M42H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU41	HA	1.00	0.004	1.00	0.33
GLU41	HB2	1.00	0.001	1.00	2.05
GLU41	HB3	1.00	0.002	1.00	2.05
GLU41	HG2	1.00	0.182	0.00	0.00
GLU41	HG3	1.00	0.002	1.00	0.42
GLU41	H	1.00	0.017	1.00	0.42
MET42	H	1.00	0.041	0.00	0.00

3.41.3 Detailed Probabilities of GLU41CG:

Overall probability: 0.860

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU41	1.00	0.86
MET42	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
E41HA	1.00
E41HB2	1.00
E41HB3	1.00
E41HG3	1.00
E41H	1.00
E41HE2	1.00
E41HG2	1.00
M42H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU41	HA	1.00	0.006	1.00	0.10
GLU41	HB2	1.00	0.027	1.00	2.24
GLU41	HB3	1.00	0.028	1.00	2.24
GLU41	HG2	1.00	0.024	1.00	17.61
GLU41	HG3	1.00	0.005	1.00	1.29
GLU41	H	1.00	0.002	1.00	0.21
MET42	H	0.98	0.056	0.02	0.00

3.41.4 Detailed Probabilities of GLU41N:

Overall probability: 0.847

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS40	0.84	1.00
GLU41	1.00	1.00
MET42	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K40HG3	0.97
K40HB2	1.00
K40HA	1.00
K40H	1.00
K40HB3	1.00
K40HG2	0.98
E41HA	1.00
E41HB2	1.00
E41HB3	1.00
E41HG2	1.00
E41HG3	1.00
E41H	1.00
M42H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS40	HA	1.00	0.010	1.00	-287422.00
LYS40	HB2	1.00	0.038	0.20	0.00
LYS40	HB3	1.00	0.007	1.00	-1920456.00
LYS40	HG2	0.98	0.024	1.00	-132344.00
LYS40	HG3	0.97	0.035	0.50	0.00
LYS40	H	1.00	0.007	1.00	-1015424.00
LYS40	HD2	0.59	0.026	1.00	-170243.00
LYS40	HD3	0.62	0.025	1.00	-170243.00
GLU41	HA	1.00	0.002	1.00	-511714.00
GLU41	HB2	1.00	0.002	1.00	-1920456.00
GLU41	HB3	1.00	0.003	1.00	-1920456.00
GLU41	HG2	1.00	0.002	1.00	-469794.00
GLU41	HG3	1.00	0.002	1.00	-638438.00
GLU41	H	1.00	0.008	1.00	-6036754.00
MET42	H	1.00	0.050	0.00	0.00

3.41.5 Detailed Probabilities of GLU41HA:

Overall probability: 0.700

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS40	0.50	1.00
GLU41	0.83	1.00
MET42	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K40HA	1.00
E41HB2	1.00
E41HB3	1.00
E41HG2	1.00
E41HG3	1.00
E41H	1.00
E41HA	1.00
M42HA	1.00
M42H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS40	HA	1.00	0.221	0.00	0.00
LYS40	H	0.87	0.012	1.00	-98765.00
GLU41	HA	1.00	0.019	1.00	12.17
GLU41	HB2	1.00	0.004	1.00	0.33
GLU41	HB3	1.00	0.004	1.00	0.33
GLU41	HG2	1.00	0.006	1.00	0.10
GLU41	HG3	1.00	0.353	0.00	0.00
GLU41	H	1.00	0.002	1.00	-511714.00
MET42	HA	1.00	0.083	0.00	0.00
MET42	H	1.00	0.006	1.00	-173560.00

3.41.6 Detailed Probabilities of GLU41HB2:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU41	1.00	0.86
MET42	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E41HA	1.00
E41HB3	1.00
E41HG2	1.00
E41HG3	1.00
E41H	1.00
E41HE2	1.00
E41HB2	1.00
M42H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU41	HA	1.00	0.030	1.00	0.00
GLU41	HB2	1.00	0.002	1.00	2.05
GLU41	HB3	1.00	0.002	1.00	2.05
GLU41	HG2	1.00	0.028	1.00	2.24
GLU41	HG3	1.00	0.002	1.00	0.66
GLU41	H	1.00	0.003	1.00	-1920456.00
MET42	H	1.00	0.004	1.00	-985493.00

3.41.7 Detailed Probabilities of GLU41HB3:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU41	1.00	0.86
MET42	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E41HA	1.00
E41HB2	1.00
E41HG2	1.00
E41HG3	1.00
E41H	1.00
E41HE2	1.00
E41HB3	1.00
M42H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU41	HA	1.00	0.030	1.00	0.00
GLU41	HB2	1.00	0.002	1.00	2.05
GLU41	HB3	1.00	0.002	1.00	2.05
GLU41	HG2	1.00	0.028	1.00	2.24
GLU41	HG3	1.00	0.002	1.00	0.66
GLU41	H	1.00	0.003	1.00	-1920456.00
MET42	H	1.00	0.004	1.00	-985493.00

3.41.8 Detailed Probabilities of GLU41HG2:

Overall probability: 0.431

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU41	0.50	0.86
MET42	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
E41HA	1.00
E41HB2	1.00
E41HB3	1.00
E41HG3	1.00
E41H	1.00
E41HE2	1.00
E41HG2	1.00
M42H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU41	HA	1.00	0.015	1.00	0.32
GLU41	HB2	1.00	0.182	0.00	0.00
GLU41	HB3	1.00	0.182	0.00	0.00
GLU41	HG2	1.00	0.024	1.00	17.61
GLU41	HG3	1.00	0.182	0.00	0.00
GLU41	H	1.00	0.002	1.00	-469794.00
MET42	H	0.98	0.052	0.02	0.00

3.41.9 Detailed Probabilities of GLU41HG3:

Overall probability: 0.857

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU41	0.83	0.86
MET42	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E41HA	1.00
E41HB2	1.00
E41HB3	1.00
E41HG2	1.00
E41H	1.00
E41HE2	1.00
E41HG3	1.00
M42H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU41	HA	1.00	0.009	1.00	0.20
GLU41	HB2	1.00	0.002	1.00	0.42
GLU41	HB3	1.00	0.002	1.00	0.42
GLU41	HG2	1.00	0.005	1.00	1.29
GLU41	HG3	1.00	0.508	0.00	0.00
GLU41	H	1.00	0.002	1.00	-638438.00
MET42	H	0.97	0.001	1.00	-85959.00

3.41.10 Detailed Probabilities of GLU41H:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS40	0.75	1.00
GLU41	1.00	1.00
MET42	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K40HG3	0.97
K40HB2	1.00
K40HA	1.00
K40H	1.00
K40HB3	1.00
K40HG2	0.98
E41HA	1.00
E41HB2	1.00
E41HB3	1.00
E41HG2	1.00
E41HG3	1.00
E41H	1.00
M42H	1.00

NOESY contacts detailed probability

3.41 GLU(41)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS40	HA	1.00	0.015	1.00	0.28
LYS40	HB2	1.00	0.096	0.00	0.00
LYS40	HB3	1.00	0.184	0.00	0.00
LYS40	HG2	0.98	0.001	1.00	0.13
LYS40	HG3	0.97	0.014	1.00	0.07
LYS40	H	1.00	0.007	1.00	-980247.00
LYS40	HD2	0.59	0.011	1.00	0.29
LYS40	HD3	0.62	0.011	1.00	0.29
GLU41	HA	1.00	0.011	1.00	0.43
GLU41	HB2	1.00	0.017	1.00	0.42
GLU41	HB3	1.00	0.017	1.00	0.42
GLU41	HG2	1.00	0.002	1.00	0.21
GLU41	HG3	1.00	0.010	1.00	0.23
GLU41	H	1.00	0.008	1.00	-6036754.00
MET42	H	1.00	0.055	0.00	0.00

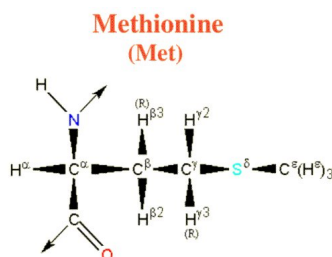


Figure 41: Image from the BMRB

Residue probability: 0.752
 Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	179.185	176.360	2.004	0.000	0.000
CA 3.42.1	57.054	56.303	4.222	0.449	1.000
CB 3.42.2	31.254	33.217	4.564	0.880	1.000
CG 3.42.3	32.468	32.123	4.122	0.881	1.000
CE 3.42.4	17.857	17.286	5.508	0.839	1.000
N 3.42.5	118.114	120.023	5.158	0.848	1.000
HA 3.42.6	4.383	4.409	0.504	0.700	1.000
HB2 3.42.7	2.191	2.016	0.340	0.778	1.000
HB3 3.42.8	1.950	1.978	0.359	0.629	1.000
HG2 3.42.9	2.656	2.410	0.360	1.000	1.000
HG3 3.42.10	2.761	2.378	0.386	1.000	1.000
HE 3.42.11	1.866	1.877	0.381	0.628	1.000
H 3.42.12	8.779	8.269	0.585	0.388	1.000

3.42.1 Detailed Probabilities of MET42CA:

Overall probability: 0.449
 Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU41	0.00	1.00
MET42	0.38	1.00
LYS43	0.90	1.00

Expected NOESY Contacts

Proton	Expected probability
E41HA	1.00
M42HB2	1.00
M42HB3	1.00
M42HG2	1.00
M42HG3	1.00
M42H	1.00
M42HA	1.00
K43H	1.00
K43HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU41	HA	1.00	0.083	0.00	0.00
MET42	HA	1.00	0.203	0.00	0.00
MET42	HB2	1.00	0.291	0.00	0.00
MET42	HB3	1.00	0.050	0.00	0.00
MET42	HG2	1.00	0.012	1.00	0.25
MET42	HG3	1.00	0.002	1.00	0.16
MET42	H	1.00	0.148	0.00	0.00
MET42	HE1	0.69	0.034	0.69	0.00
LYS43	HA	1.00	0.032	0.80	0.00
LYS43	H	1.00	0.002	1.00	0.17

3.42.2 Detailed Probabilities of MET42CB:

Overall probability: 0.880

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET42	0.86	1.00
LYS43	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
M42HA	1.00
M42HB3	1.00
M42HG2	1.00
M42HG3	1.00
M42HE1	0.96
M42H	1.00
M42HB2	1.00
K43H	1.00

NOESY contacts detailed probability

3.42 MET(42)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET42	HA	1.00	0.014	1.00	0.24
MET42	HB2	1.00	0.006	1.00	1.64
MET42	HB3	1.00	0.000	1.00	1.07
MET42	HG2	1.00	0.005	1.00	0.26
MET42	HG3	1.00	0.002	1.00	0.32
MET42	HE1	0.96	0.084	0.04	0.00
MET42	H	1.00	0.003	1.00	0.25
LYS43	H	1.00	0.003	1.00	0.18

3.42.3 Detailed Probabilities of MET42CG:

Overall probability: 0.881

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET42	1.00	1.00
LYS43	0.05	1.00

Expected NOESY Contacts

Proton	Expected probability
M42HA	1.00
M42HB2	1.00
M42HB3	1.00
M42HG2	1.00
M42HE1	1.00
M42H	1.00
M42HG3	1.00
K43H	0.95

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET42	HA	1.00	0.010	1.00	0.16
MET42	HB2	1.00	0.008	1.00	0.32
MET42	HB3	1.00	0.003	1.00	0.32
MET42	HG2	1.00	0.012	1.00	1.24
MET42	HG3	1.00	0.005	1.00	1.63
MET42	HE1	1.00	0.021	1.00	0.28
MET42	H	1.00	0.004	1.00	0.21
LYS43	H	0.95	1.284	0.05	0.00

3.42.4 Detailed Probabilities of MET42CE:

Overall probability: 0.839

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET42	0.84	1.00

Expected NOESY Contacts

Proton	Expected probability
M42HB2	0.96
M42HB3	0.97
M42HG2	1.00
M42HG3	1.00
M42HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET42	HB2	0.96	0.006	1.00	0.51
MET42	HB3	0.97	0.054	0.03	0.00
MET42	HG2	1.00	0.011	1.00	0.72
MET42	HG3	1.00	0.004	1.00	0.64
MET42	HE1	1.00	0.006	1.00	77.74
MET42	HA	0.67	0.012	1.00	0.83

3.42.5 Detailed Probabilities of MET42N:

Overall probability: 0.848

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU41	0.67	1.00
MET42	1.00	1.00
LYS43	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E41HB2	1.00
E41HA	1.00
E41HG3	0.97
E41HB3	1.00
E41H	1.00
E41HG2	0.98
M42HA	1.00
M42HB2	1.00
M42HB3	1.00
M42HG2	1.00
M42HG3	1.00
M42H	1.00
K43H	1.00

NOESY contacts detailed probability

3.42 MET(42)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU41	HA	1.00	0.006	1.00	-173560.00
GLU41	HB2	1.00	0.005	1.00	-985493.00
GLU41	HB3	1.00	0.004	1.00	-985493.00
GLU41	HG2	0.98	0.052	0.02	0.00
GLU41	HG3	0.97	0.001	1.00	-85959.00
GLU41	H	1.00	0.055	0.00	0.00
MET42	HA	1.00	0.008	1.00	-508699.00
MET42	HB2	1.00	0.006	1.00	-668680.00
MET42	HB3	1.00	0.005	1.00	-985493.00
MET42	HG2	1.00	0.012	1.00	-683399.00
MET42	HG3	1.00	0.015	1.00	-514047.00
MET42	H	1.00	0.003	1.00	-5463178.00
LYS43	H	1.00	0.000	1.00	-851096.00

3.42.6 Detailed Probabilities of MET42HA:

Overall probability: 0.700

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU41	0.00	1.00
MET42	0.71	1.00
LYS43	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E41HA	1.00
M42HB2	1.00
M42HB3	1.00
M42HG2	1.00
M42HG3	1.00
M42H	1.00
M42HA	1.00
K43H	1.00
K43HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU41	HA	1.00	0.101	0.00	0.00
MET42	HA	1.00	0.203	0.00	0.00
MET42	HB2	1.00	0.014	1.00	0.24
MET42	HB3	1.00	1.624	0.00	0.00
MET42	HG2	1.00	0.027	1.00	0.07
MET42	HG3	1.00	0.010	1.00	0.16
MET42	H	1.00	0.008	1.00	-508699.00
MET42	HE1	0.69	0.012	1.00	0.83
LYS43	HA	1.00	0.001	1.00	0.14
LYS43	H	1.00	0.009	1.00	-243082.00

3.42.7 Detailed Probabilities of MET42HB2:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET42	0.71	1.00
LYS43	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
M42HA	1.00
M42HB3	1.00
M42HG2	1.00
M42HG3	1.00
M42HE1	0.96
M42H	1.00
M42HB2	1.00
K43H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET42	HA	1.00	0.291	0.00	0.00
MET42	HB2	1.00	0.006	1.00	1.64
MET42	HB3	1.00	0.324	0.00	0.00
MET42	HG2	1.00	0.002	1.00	0.26
MET42	HG3	1.00	0.008	1.00	0.32
MET42	HE1	0.96	0.006	1.00	0.51
MET42	H	1.00	0.006	1.00	-668680.00
LYS43	H	1.00	0.006	1.00	-362573.00
LYS43	HA	0.68	0.026	1.00	2.61

3.42.8 Detailed Probabilities of MET42HB3:

Overall probability: 0.629

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET42	0.58	1.00
LYS43	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
M42HA	1.00
M42HB2	1.00
M42HG2	1.00
M42HG3	1.00
M42HE1	0.97
M42H	1.00
M42HB3	1.00
K43H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET42	HA	1.00	0.050	0.00	0.00
MET42	HB2	1.00	0.000	1.00	1.07
MET42	HB3	1.00	0.565	0.00	0.00
MET42	HG2	1.00	0.021	1.00	0.26
MET42	HG3	1.00	0.003	1.00	0.32
MET42	HE1	0.97	0.054	0.03	0.00
MET42	H	1.00	0.005	1.00	-985493.00
LYS43	H	1.00	0.025	1.00	-2484232.00

3.42.9 Detailed Probabilities of MET42HG2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET42	1.00	1.00
LYS43	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
M42HA	1.00
M42HB2	1.00
M42HB3	1.00
M42HG3	1.00
M42HE1	1.00
M42H	1.00
M42HG2	1.00
K43H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET42	HA	1.00	0.012	1.00	0.25
MET42	HB2	1.00	0.005	1.00	0.26
MET42	HB3	1.00	0.025	1.00	0.86
MET42	HG2	1.00	0.009	1.00	1.42
MET42	HG3	1.00	0.012	1.00	1.24
MET42	HE1	1.00	0.011	1.00	0.72
MET42	H	1.00	0.012	1.00	-683399.00
LYS43	H	0.98	0.002	1.00	-110437.00

3.42.10 Detailed Probabilities of MET42HG3:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET42	1.00	1.00
LYS43	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
M42HA	1.00
M42HB2	1.00
M42HB3	1.00
M42HG2	1.00
M42HE1	1.00
M42H	1.00
M42HG3	1.00
K43H	0.95

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET42	HA	1.00	0.002	1.00	0.16
MET42	HB2	1.00	0.002	1.00	0.32
MET42	HB3	1.00	0.002	1.00	0.34
MET42	HG2	1.00	0.008	1.00	1.05
MET42	HG3	1.00	0.005	1.00	1.63
MET42	HE1	1.00	0.004	1.00	0.64
MET42	H	1.00	0.015	1.00	-514047.00
LYS43	H	0.95	0.003	1.00	-88180.00

3.42.11 Detailed Probabilities of MET42HE1:

Overall probability: 0.628

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET42	0.63	1.00

Expected NOESY Contacts

Proton	Expected probability
M42HB2	0.96
M42HB3	0.97
M42HG2	1.00
M42HG3	1.00
M42HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET42	HB2	0.96	0.084	0.04	0.00
MET42	HB3	0.97	0.649	0.03	0.00
MET42	HG2	1.00	0.018	1.00	0.26
MET42	HG3	1.00	0.021	1.00	0.28
MET42	HE1	1.00	0.006	1.00	77.74
MET42	HA	0.69	0.034	0.69	0.00

3.42.12 Detailed Probabilities of MET42H:

Overall probability: 0.388

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU41	0.01	1.00
MET42	0.67	1.00
LYS43	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E41HB2	1.00
E41HA	1.00
E41HG3	0.97
E41HB3	1.00
E41H	1.00
E41HG2	0.98
M42HA	1.00
M42HB2	1.00
M42HB3	1.00
M42HG2	1.00
M42HG3	1.00
M42H	1.00
K43H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU41	HA	1.00	0.047	0.00	0.00
GLU41	HB2	1.00	0.041	0.00	0.00
GLU41	HB3	1.00	0.041	0.00	0.00
GLU41	HG2	0.98	0.056	0.02	0.00
GLU41	HG3	0.97	0.048	0.03	0.00
GLU41	H	1.00	0.050	0.00	0.00
MET42	HA	1.00	0.148	0.00	0.00
MET42	HB2	1.00	0.003	1.00	0.25
MET42	HB3	1.00	1.076	0.00	0.00
MET42	HG2	1.00	0.004	1.00	0.20
MET42	HG3	1.00	0.004	1.00	0.21
MET42	H	1.00	0.003	1.00	-5463178.00
LYS43	H	1.00	0.001	1.00	-878593.00

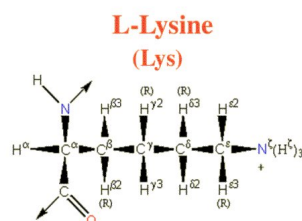


Figure 42: Image from the BMRB

Residue probability: 0.815
Residue probability confidence: 0.945

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.187	176.660	3.133	0.000	0.000
CA 3.43.1	59.390	57.014	3.028	0.771	1.000
CB 3.43.2	31.962	32.981	3.186	0.669	1.000
CG 3.43.3	24.910	24.941	1.956	0.730	0.917
CD 3.43.4	28.780	29.020	2.193	0.990	0.900
CE 3.43.5	41.780	41.893	1.492	1.000	0.889
N 3.43.6	120.740	120.954	4.210	0.941	1.000
NZ	NA	—	—	0.000	0.000
HA 3.43.7	4.088	4.262	0.489	0.754	1.000
HB2 3.43.8	1.907	1.774	0.365	0.992	1.000
HB3 3.43.9	1.901	1.742	0.385	0.925	1.000
HG2 3.43.10	1.513	1.358	0.344	0.621	0.917
HG3 3.43.11	1.370	1.343	0.357	0.522	0.917
HD2 3.43.12	1.678	1.614	0.957	0.900	0.900
HD3 3.43.13	1.683	1.595	0.387	0.900	0.900
HE2 3.43.14	2.980	2.907	0.230	0.781	0.889
HE3 3.43.15	2.975	2.901	0.241	0.780	0.889
H 3.43.16	7.499	8.185	0.605	0.769	1.000
HZ	NA	—	—	0.000	0.000

3.43.1 Detailed Probabilities of LYS43CA:

Overall probability: 0.771
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET42	1.00	1.00
LYS43	0.78	1.00
LYS44	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
M42HA	1.00
K43HB2	1.00
K43HB3	1.00
K43HG2	1.00
K43HG3	1.00
K43HD2	0.98
K43HD3	0.98
K43H	1.00
K43HA	1.00
K44HA	1.00
K44H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET42	HA	1.00	0.001	1.00	0.14
MET42	HB2	0.68	0.026	1.00	2.61
LYS43	HA	1.00	0.046	0.00	0.00
LYS43	HB2	1.00	0.005	1.00	3.96
LYS43	HB3	1.00	0.011	1.00	3.96
LYS43	HG2	1.00	0.032	0.80	0.00
LYS43	HG3	1.00	0.069	0.00	0.00
LYS43	HD2	0.98	0.008	1.00	1.91
LYS43	HD3	0.98	0.003	1.00	1.91
LYS43	H	1.00	0.014	1.00	0.89
LYS43	HE2	0.77	0.014	1.00	0.49
LYS43	HE3	0.76	0.009	1.00	0.49
LYS44	HA	1.00	0.019	1.00	41.95
LYS44	H	1.00	0.040	0.00	0.00

3.43.2 Detailed Probabilities of LYS43CB:

Overall probability: 0.669

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS43	0.60	1.00
LYS44	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K43HA	1.00
K43HB3	1.00
K43HG2	1.00
K43HG3	1.00
K43HD2	1.00
K43HD3	1.00
K43HE2	0.98
K43HE3	0.99
K43H	1.00
K43HB2	1.00
K44H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS43	HA	1.00	0.003	1.00	4.53
LYS43	HB2	1.00	0.003	1.00	53.87
LYS43	HB3	1.00	0.003	1.00	53.87
LYS43	HG2	1.00	0.040	0.00	0.00
LYS43	HG3	1.00	0.103	0.00	0.00
LYS43	HD2	1.00	0.005	1.00	5.56
LYS43	HD3	1.00	0.000	1.00	5.56
LYS43	HE2	0.98	0.051	0.02	0.00
LYS43	HE3	0.99	0.046	0.01	0.00
LYS43	H	1.00	0.026	1.00	1.72
LYS44	H	1.00	0.028	1.00	1.72
LYS44	HA	0.64	0.024	1.00	4.53

3.43.3 Detailed Probabilities of LYS43CG:

Overall probability: 0.730

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS43	0.80	0.91
LYS44	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
K43HA	1.00
K43HB2	1.00
K43HB3	1.00
K43HG3	1.00
K43HD2	1.00
K43HD3	1.00
K43HE2	1.00
K43HE3	1.00
K43H	1.00
K43HZ2	1.00
K43HG2	1.00
K44H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS43	HA	1.00	0.002	1.00	1.20
LYS43	HB2	1.00	0.010	1.00	2.42
LYS43	HB3	1.00	0.004	1.00	2.42
LYS43	HG2	1.00	0.091	0.00	0.00
LYS43	HG3	1.00	0.203	0.00	0.00
LYS43	HD2	1.00	0.004	1.00	6.34
LYS43	HD3	1.00	0.001	1.00	6.34
LYS43	HE2	1.00	0.006	1.00	0.99
LYS43	HE3	1.00	0.011	1.00	0.99
LYS43	H	1.00	0.001	1.00	0.22
LYS44	H	0.97	0.055	0.03	0.00

3.43.4 Detailed Probabilities of LYS43CD:

Overall probability: 0.990

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS43	0.99	0.90

Expected NOESY Contacts

Proton	Expected probability
K43HA	0.98
K43HB2	1.00
K43HB3	1.00
K43HG2	1.00
K43HG3	1.00
K43HD3	1.00
K43HE2	1.00
K43HE3	1.00
K43HZ2	1.00
K43HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS43	HA	0.98	0.003	1.00	1.30
LYS43	HB2	1.00	0.025	1.00	5.45
LYS43	HB3	1.00	0.031	0.90	0.00
LYS43	HG2	1.00	0.016	1.00	11.42
LYS43	HG3	1.00	0.008	1.00	0.81
LYS43	HD2	1.00	0.006	1.00	244.35
LYS43	HD3	1.00	0.001	1.00	244.35
LYS43	HE2	1.00	0.002	1.00	6.07
LYS43	HE3	1.00	0.007	1.00	6.07
LYS43	H	0.88	0.019	1.00	0.33

3.43.5 Detailed Probabilities of LYS43CE:

Overall probability: 1.000

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS43	1.00	0.89

Expected NOESY Contacts

Proton	Expected probability
K43HB2	0.98
K43HB3	0.99
K43HG2	1.00
K43HG3	1.00
K43HD2	1.00
K43HD3	1.00
K43HE3	1.00
K43HZ2	1.00
K43HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS43	HB2	0.98	0.023	1.00	1.41
LYS43	HB3	0.99	0.029	1.00	1.41
LYS43	HG2	1.00	0.021	1.00	3.64
LYS43	HG3	1.00	0.029	1.00	2.36
LYS43	HD2	1.00	0.018	1.00	15.02
LYS43	HD3	1.00	0.013	1.00	15.02
LYS43	HE2	1.00	0.007	1.00	641.65
LYS43	HE3	1.00	0.012	1.00	641.65
LYS43	HA	0.77	0.023	1.00	0.98

3.43.6 Detailed Probabilities of LYS43N:

Overall probability: 0.941

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET42	1.00	1.00
LYS43	1.00	1.00
LYS44	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
M42HA	1.00
M42H	1.00
M42HG3	0.95
M42HB2	1.00
M42HB3	1.00
M42HG2	0.98
K43HA	1.00
K43HB2	1.00
K43HB3	1.00
K43HG2	1.00
K43HG3	1.00
K43H	1.00
K44H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET42	HA	1.00	0.009	1.00	-243082.00
MET42	HB2	1.00	0.006	1.00	-362573.00
MET42	HB3	1.00	0.025	1.00	-2484232.00
MET42	HG2	0.98	0.002	1.00	-110437.00
MET42	HG3	0.95	0.003	1.00	-88180.00
MET42	H	1.00	0.001	1.00	-878593.00
LYS43	HA	1.00	0.002	1.00	-1013474.00
LYS43	HB2	1.00	0.018	1.00	-2484232.00
LYS43	HB3	1.00	0.024	1.00	-2484232.00
LYS43	HG2	1.00	0.008	1.00	-405292.00
LYS43	HG3	1.00	0.011	1.00	-264404.00
LYS43	H	1.00	0.001	1.00	-9411694.00
LYS43	HD2	0.88	0.012	1.00	-325852.00
LYS43	HD3	0.87	0.007	1.00	-325852.00
LYS44	H	1.00	0.055	0.00	0.00
LYS44	HA	0.88	0.025	1.00	-1013474.00
LYS44	HB2	0.61	0.014	1.00	-2484232.00

3.43.7 Detailed Probabilities of LYS43HA:

Overall probability: 0.754

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET42	0.80	1.00
LYS43	0.80	1.00
LYS44	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
M42HA	1.00
K43HB2	1.00
K43HB3	1.00
K43HG2	1.00
K43HG3	1.00
K43HD2	0.98
K43HD3	0.98
K43H	1.00
K43HA	1.00
K44HA	1.00
K44H	1.00

NOESY contacts detailed probability

3.43 LYS(43)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET42	HA	1.00	0.032	0.80	0.00
LYS43	HA	1.00	0.046	0.00	0.00
LYS43	HB2	1.00	0.003	1.00	4.53
LYS43	HB3	1.00	0.003	1.00	4.53
LYS43	HG2	1.00	0.002	1.00	1.20
LYS43	HG3	1.00	0.051	0.00	0.00
LYS43	HD2	0.98	0.003	1.00	1.30
LYS43	HD3	0.98	0.003	1.00	1.30
LYS43	H	1.00	0.002	1.00	-1013474.00
LYS43	HE2	0.77	0.023	1.00	0.98
LYS43	HE3	0.76	0.023	1.00	0.98
LYS44	HA	1.00	0.046	0.00	0.00
LYS44	H	1.00	0.028	1.00	-1290945.00

3.43.8 Detailed Probabilities of LYS43HB2:

Overall probability: 0.992

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS43	0.99	1.00
LYS44	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K43HA	1.00
K43HB3	1.00
K43HG2	1.00
K43HG3	1.00
K43HD2	1.00
K43HD3	1.00
K43HE2	0.98
K43HE3	0.99
K43H	1.00
K43HB2	1.00
K44H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS43	HA	1.00	0.005	1.00	3.96
LYS43	HB2	1.00	0.003	1.00	53.87
LYS43	HB3	1.00	0.003	1.00	53.87
LYS43	HG2	1.00	0.010	1.00	2.42
LYS43	HG3	1.00	0.031	0.90	0.00
LYS43	HD2	1.00	0.025	1.00	5.45
LYS43	HD3	1.00	0.025	1.00	5.45
LYS43	HE2	0.98	0.023	1.00	1.41
LYS43	HE3	0.99	0.023	1.00	1.41
LYS43	H	1.00	0.018	1.00	-2484232.00
LYS44	H	1.00	0.001	1.00	-2953164.00
LYS44	HA	0.64	0.005	1.00	3.96

3.43.9 Detailed Probabilities of LYS43HB3:

Overall probability: 0.925

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS43	0.91	1.00
LYS44	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K43HA	1.00
K43HB2	1.00
K43HG2	1.00
K43HG3	1.00
K43HD2	1.00
K43HD3	1.00
K43HE2	0.99
K43HE3	0.99
K43H	1.00
K43HB3	1.00
K44H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS43	HA	1.00	0.011	1.00	3.96
LYS43	HB2	1.00	0.003	1.00	53.87
LYS43	HB3	1.00	0.003	1.00	53.87
LYS43	HG2	1.00	0.004	1.00	2.42
LYS43	HG3	1.00	0.037	0.30	0.00
LYS43	HD2	1.00	0.031	0.90	0.00
LYS43	HD3	1.00	0.031	0.90	0.00
LYS43	HE2	0.99	0.029	1.00	1.41
LYS43	HE3	0.99	0.029	1.00	1.41
LYS43	H	1.00	0.024	1.00	-2484232.00
LYS44	H	1.00	0.007	1.00	-2953164.00
LYS44	HA	0.82	0.011	1.00	3.96

3.43.10 Detailed Probabilities of LYS43HG2:

Overall probability: 0.621

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS43	0.68	0.91
LYS44	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
K43HA	1.00
K43HB2	1.00
K43HB3	1.00
K43HG3	1.00
K43HD2	1.00
K43HD3	1.00
K43HE2	1.00
K43HE3	1.00
K43H	1.00
K43HZ2	1.00
K43HG2	1.00
K44H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS43	HA	1.00	0.032	0.80	0.00
LYS43	HB2	1.00	0.040	0.00	0.00
LYS43	HB3	1.00	0.040	0.00	0.00
LYS43	HG2	1.00	0.091	0.00	0.00
LYS43	HG3	1.00	0.019	1.00	4.89
LYS43	HD2	1.00	0.016	1.00	11.42
LYS43	HD3	1.00	0.016	1.00	11.42
LYS43	HE2	1.00	0.021	1.00	3.64
LYS43	HE3	1.00	0.021	1.00	3.64
LYS43	H	1.00	0.008	1.00	-405292.00
LYS44	H	0.97	0.073	0.03	0.00

3.43.11 Detailed Probabilities of LYS43HG3:

Overall probability: 0.522

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS43	0.57	0.91
LYS44	0.04	1.00

Expected NOESY Contacts

Proton	Expected probability
K43HA	1.00
K43HB2	1.00
K43HB3	1.00
K43HG2	1.00
K43HD2	1.00
K43HD3	1.00
K43HE2	1.00
K43HE3	1.00
K43H	1.00
K43HZ2	1.00
K43HG3	1.00
K44H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS43	HA	1.00	0.069	0.00	0.00
LYS43	HB2	1.00	0.103	0.00	0.00
LYS43	HB3	1.00	0.103	0.00	0.00
LYS43	HG2	1.00	0.203	0.00	0.00
LYS43	HG3	1.00	0.014	1.00	36.93
LYS43	HD2	1.00	0.008	1.00	0.81
LYS43	HD3	1.00	0.033	0.70	0.00
LYS43	HE2	1.00	0.029	1.00	2.36
LYS43	HE3	1.00	0.029	1.00	2.36
LYS43	H	1.00	0.011	1.00	-264404.00
LYS44	H	0.96	0.067	0.04	0.00

3.43.12 Detailed Probabilities of LYS43HD2:

Overall probability: 0.900

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS43	0.90	0.90

Expected NOESY Contacts

Proton	Expected probability
K43HA	0.98
K43HB2	1.00
K43HB3	1.00
K43HG2	1.00
K43HG3	1.00
K43HD3	1.00
K43HE2	1.00
K43HE3	1.00
K43HZ2	1.00
K43HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS43	HA	0.98	0.008	1.00	1.91
LYS43	HB2	1.00	0.005	1.00	5.56
LYS43	HB3	1.00	0.005	1.00	5.56
LYS43	HG2	1.00	0.004	1.00	6.34
LYS43	HG3	1.00	0.043	0.00	0.00
LYS43	HD2	1.00	0.006	1.00	244.35
LYS43	HD3	1.00	0.006	1.00	244.35
LYS43	HE2	1.00	0.018	1.00	15.02
LYS43	HE3	1.00	0.018	1.00	15.02
LYS43	H	0.88	0.012	1.00	-325852.00

3.43.13 Detailed Probabilities of LYS43HD3:

Overall probability: 0.900

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS43	0.90	0.90

Expected NOESY Contacts

Proton	Expected probability
K43HA	0.98
K43HB2	1.00
K43HB3	1.00
K43HG2	1.00
K43HG3	1.00
K43HD2	1.00
K43HE2	1.00
K43HE3	1.00
K43HZ2	1.00
K43HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS43	HA	0.98	0.003	1.00	1.91
LYS43	HB2	1.00	0.000	1.00	5.56
LYS43	HB3	1.00	0.000	1.00	5.56
LYS43	HG2	1.00	0.001	1.00	6.34
LYS43	HG3	1.00	0.048	0.00	0.00
LYS43	HD2	1.00	0.001	1.00	244.35
LYS43	HD3	1.00	0.001	1.00	244.35
LYS43	HE2	1.00	0.013	1.00	15.02
LYS43	HE3	1.00	0.013	1.00	15.02
LYS43	H	0.87	0.007	1.00	-325852.00

3.43.14 Detailed Probabilities of LYS43HE2:

Overall probability: 0.781

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS43	0.78	0.89

Expected NOESY Contacts

Proton	Expected probability
K43HB2	0.98
K43HB3	0.99
K43HG2	1.00
K43HG3	1.00
K43HD2	1.00
K43HD3	1.00
K43HE3	1.00
K43HZ2	1.00
K43HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS43	HB2	0.98	0.051	0.02	0.00
LYS43	HB3	0.99	0.051	0.01	0.00
LYS43	HG2	1.00	0.006	1.00	0.99
LYS43	HG3	1.00	0.006	1.00	1.13
LYS43	HD2	1.00	0.002	1.00	6.07
LYS43	HD3	1.00	0.002	1.00	6.07
LYS43	HE2	1.00	0.007	1.00	641.65
LYS43	HE3	1.00	0.007	1.00	641.65
LYS43	HA	0.77	0.014	1.00	0.49

3.43.15 Detailed Probabilities of LYS43HE3:

Overall probability: 0.780

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS43	0.78	0.89

Expected NOESY Contacts

Proton	Expected probability
K43HB2	0.99
K43HB3	0.99
K43HG2	1.00
K43HG3	1.00
K43HD2	1.00
K43HD3	1.00
K43HE2	1.00
K43HZ2	1.00
K43HE3	1.00

NOESY contacts detailed probability

3.43 LYS(43)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS43	HB2	0.99	0.046	0.01	0.00
LYS43	HB3	0.99	0.046	0.01	0.00
LYS43	HG2	1.00	0.011	1.00	0.99
LYS43	HG3	1.00	0.001	1.00	1.13
LYS43	HD2	1.00	0.007	1.00	6.07
LYS43	HD3	1.00	0.007	1.00	6.07
LYS43	HE2	1.00	0.012	1.00	641.65
LYS43	HE3	1.00	0.012	1.00	641.65
LYS43	HA	0.76	0.009	1.00	0.49

3.43.16 Detailed Probabilities of LYS43H:

Overall probability: 0.769

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET42	0.51	1.00
LYS43	1.00	1.00
LYS44	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
M42HA	1.00
M42H	1.00
M42HG3	0.95
M42HB2	1.00
M42HB3	1.00
M42HG2	0.98
K43HA	1.00
K43HB2	1.00
K43HB3	1.00
K43HG2	1.00
K43HG3	1.00
K43H	1.00
K44H	1.00

NOESY contacts detailed probability

3.43 LYS(43)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET42	HA	1.00	0.002	1.00	0.17
MET42	HB2	1.00	0.003	1.00	0.18
MET42	HB3	1.00	0.901	0.00	0.00
MET42	HG2	0.98	1.284	0.02	0.00
MET42	HG3	0.95	1.284	0.05	0.00
MET42	H	1.00	0.000	1.00	-851096.00
LYS43	HA	1.00	0.014	1.00	0.89
LYS43	HB2	1.00	0.026	1.00	1.72
LYS43	HB3	1.00	0.026	1.00	1.72
LYS43	HG2	1.00	0.001	1.00	0.22
LYS43	HG3	1.00	0.005	1.00	0.17
LYS43	H	1.00	0.001	1.00	-9411694.00
LYS43	HD2	0.88	0.019	1.00	0.33
LYS43	HD3	0.87	0.019	1.00	0.33
LYS44	H	1.00	0.049	0.00	0.00
LYS44	HA	0.88	0.014	1.00	0.89
LYS44	HB2	0.61	0.026	1.00	1.72

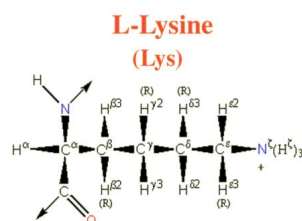


Figure 43: Image from the BMRB

Residue probability: 0.845
Residue probability confidence: 0.942

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	179.601	176.660	3.133	0.000	0.000
CA 3.44.1	59.500	57.014	3.028	0.687	1.000
CB 3.44.2	32.070	32.981	3.186	0.950	1.000
CG 3.44.3	24.910	24.941	1.956	0.989	0.900
CD 3.44.4	29.133	29.020	2.193	0.813	0.889
CE 3.44.5	41.780	41.893	1.492	0.825	0.875
N 3.44.6	118.269	120.954	4.210	0.837	1.000
NZ	NA	—	—	0.000	0.000
HA 3.44.7	4.061	4.262	0.489	0.933	1.000
HB2 3.44.8	1.911	1.774	0.365	1.000	1.000
HB3 3.44.9	1.906	1.742	0.385	1.000	1.000
HG2 3.44.10	1.582	1.358	0.344	0.633	0.909
HG3 3.44.11	1.438	1.343	0.357	0.767	0.900
HD2 3.44.12	1.700	1.614	0.957	0.822	0.889
HD3 3.44.13	1.702	1.595	0.387	0.800	0.889
HE 3.44.14	2.930	2.907	0.230	1.000	0.875
H 3.44.15	7.445	8.185	0.605	0.621	1.000
HZ	NA	—	—	0.000	0.000

3.44.1 Detailed Probabilities of LYS44CA:

Overall probability: 0.687
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS43	0.75	1.00
LYS44	0.81	1.00
LEU45	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K43HA	1.00
K44HB2	1.00
K44HB3	1.00
K44HG2	1.00
K44HG3	1.00
K44HD2	0.98
K44HD3	0.98
K44H	1.00
K44HA	1.00
L45HA	1.00
L45H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS43	HA	1.00	0.046	0.00	0.00
LYS43	HB2	0.64	0.005	1.00	3.96
LYS43	HB3	0.82	0.011	1.00	3.96
LYS43	H	0.88	0.014	1.00	0.89
LYS44	HA	1.00	0.019	1.00	41.95
LYS44	HB2	1.00	0.001	1.00	3.96
LYS44	HB3	1.00	0.006	1.00	3.96
LYS44	HG2	1.00	0.037	0.30	0.00
LYS44	HG3	1.00	0.001	1.00	1.07
LYS44	HD2	0.98	0.014	1.00	1.91
LYS44	HD3	0.98	0.016	1.00	1.91
LYS44	H	1.00	0.040	0.00	0.00
LYS44	HE2	0.77	0.007	1.00	0.40
LEU45	HA	1.00	0.106	0.00	0.00
LEU45	H	1.00	0.069	0.00	0.00

3.44.2 Detailed Probabilities of LYS44CB:

Overall probability: 0.950

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS44	0.94	1.00
LEU45	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K44HA	1.00
K44HB3	1.00
K44HG2	1.00
K44HG3	1.00
K44HD2	1.00
K44HD3	1.00
K44HE2	0.98
K44H	1.00
K44HB2	1.00
L45H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS44	HA	1.00	0.024	1.00	4.53
LYS44	HB2	1.00	0.007	1.00	53.87
LYS44	HB3	1.00	0.002	1.00	53.87
LYS44	HG2	1.00	0.001	1.00	3.20
LYS44	HG3	1.00	0.035	0.50	0.00
LYS44	HD2	1.00	0.017	1.00	5.56
LYS44	HD3	1.00	0.019	1.00	5.56
LYS44	HE2	0.98	0.001	1.00	0.70
LYS44	H	1.00	0.028	1.00	1.72
LEU45	H	1.00	0.001	1.00	0.64

3.44.3 Detailed Probabilities of LYS44CG:

Overall probability: 0.989

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS44	0.99	0.90

Expected NOESY Contacts

Proton	Expected probability
K44HA	1.00
K44HB2	1.00
K44HB3	1.00
K44HG2	1.00
K44HD2	1.00
K44HD3	1.00
K44HE2	1.00
K44H	1.00
K44HZ2	1.00
K44HG3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS44	HA	1.00	0.027	1.00	0.93
LYS44	HB2	1.00	0.019	1.00	2.94
LYS44	HB3	1.00	0.014	1.00	2.94
LYS44	HG2	1.00	0.010	1.00	8.71
LYS44	HG3	1.00	0.031	0.90	0.00
LYS44	HD2	1.00	0.013	1.00	6.92
LYS44	HD3	1.00	0.015	1.00	6.92
LYS44	HE2	1.00	0.030	1.00	0.86
LYS44	H	1.00	0.010	1.00	0.23

3.44.4 Detailed Probabilities of LYS44CD:

Overall probability: 0.813

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS44	0.81	0.89

Expected NOESY Contacts

Proton	Expected probability
K44HA	0.98
K44HB2	1.00
K44HB3	1.00
K44HG2	1.00
K44HG3	1.00
K44HD3	1.00
K44HE2	1.00
K44HZ2	1.00
K44HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS44	HA	0.98	0.013	1.00	1.33
LYS44	HB2	1.00	0.021	1.00	5.45
LYS44	HB3	1.00	0.026	1.00	5.45
LYS44	HG2	1.00	0.085	0.00	0.00
LYS44	HG3	1.00	0.035	0.50	0.00
LYS44	HD2	1.00	0.016	1.00	244.35
LYS44	HD3	1.00	0.018	1.00	244.35
LYS44	HE2	1.00	0.017	1.00	4.26

3.44.5 Detailed Probabilities of LYS44CE:

Overall probability: 0.825

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS44	0.82	0.88

Expected NOESY Contacts

Proton	Expected probability
K44HB2	0.98
K44HB3	0.99
K44HG2	1.00
K44HG3	1.00
K44HD2	1.00
K44HD3	1.00
K44HE3	1.00
K44HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS44	HB2	0.99	0.004	1.00	1.28
LYS44	HB3	0.99	0.009	1.00	1.28
LYS44	HG2	1.00	0.022	1.00	1.96
LYS44	HG3	1.00	0.027	1.00	1.85
LYS44	HD2	1.00	0.036	0.40	0.00
LYS44	HD3	1.00	0.038	0.20	0.00
LYS44	HE2	1.00	0.013	1.00	220.78
LYS44	HA	0.76	0.004	1.00	0.98

3.44.6 Detailed Probabilities of LYS44N:

Overall probability: 0.837

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS43	0.63	1.00
LYS44	1.00	1.00
LEU45	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K43HB2	1.00
K43HG3	0.96
K43HB3	1.00
K43HA	1.00
K43HG2	0.97
K43H	1.00
K44HA	1.00
K44HB2	1.00
K44HB3	1.00
K44HG2	1.00
K44HG3	1.00
K44H	1.00
L45H	1.00

NOESY contacts detailed probability

3.44 LYS(44)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS43	HA	1.00	0.028	1.00	-1290945.00
LYS43	HB2	1.00	0.001	1.00	-2953164.00
LYS43	HB3	1.00	0.007	1.00	-2953164.00
LYS43	HG2	0.97	0.073	0.03	0.00
LYS43	HG3	0.96	0.067	0.04	0.00
LYS43	H	1.00	0.049	0.00	0.00
LYS43	HD2	0.56	0.011	1.00	-421987.00
LYS43	HD3	0.59	0.006	1.00	-421987.00
LYS44	HA	1.00	0.001	1.00	-1290945.00
LYS44	HB2	1.00	0.003	1.00	-2953164.00
LYS44	HB3	1.00	0.002	1.00	-2953164.00
LYS44	HG2	1.00	0.004	1.00	-855885.00
LYS44	HG3	1.00	0.001	1.00	-383812.00
LYS44	H	1.00	0.005	1.00	-10036825.00
LYS44	HD2	0.88	0.011	1.00	-421987.00
LYS44	HD3	0.87	0.013	1.00	-421987.00
LEU45	H	1.00	0.003	1.00	-961380.00
LEU45	HB2	0.61	0.004	1.00	-2953164.00

3.44.7 Detailed Probabilities of LYS44HA:

Overall probability: 0.933

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS43	1.00	1.00
LYS44	1.00	1.00
LEU45	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K43HA	1.00
K44HB2	1.00
K44HB3	1.00
K44HG2	1.00
K44HG3	1.00
K44HD2	0.98
K44HD3	0.98
K44H	1.00
K44HA	1.00
L45HA	1.00
L45H	1.00

NOESY contacts detailed probability

3.44 LYS(44)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS43	HA	1.00	0.019	1.00	41.95
LYS43	HB2	0.64	0.024	1.00	4.53
LYS43	HB3	0.82	0.024	1.00	4.53
LYS43	H	0.88	0.025	1.00	-1013474.00
LYS44	HA	1.00	0.019	1.00	41.95
LYS44	HB2	1.00	0.024	1.00	4.53
LYS44	HB3	1.00	0.024	1.00	4.53
LYS44	HG2	1.00	0.024	1.00	0.75
LYS44	HG3	1.00	0.027	1.00	0.93
LYS44	HD2	0.98	0.013	1.00	1.33
LYS44	HD3	0.98	0.013	1.00	1.33
LYS44	H	1.00	0.001	1.00	-1290945.00
LYS44	HE2	0.77	0.004	1.00	0.98
LEU45	HA	1.00	0.122	0.00	0.00
LEU45	H	1.00	0.003	1.00	-320505.00

3.44.8 Detailed Probabilities of LYS44HB2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS44	1.00	1.00
LEU45	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K44HA	1.00
K44HB3	1.00
K44HG2	1.00
K44HG3	1.00
K44HD2	1.00
K44HD3	1.00
K44HE2	0.98
K44H	1.00
K44HB2	1.00
L45H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS44	HA	1.00	0.001	1.00	3.96
LYS44	HB2	1.00	0.007	1.00	53.87
LYS44	HB3	1.00	0.007	1.00	53.87
LYS44	HG2	1.00	0.007	1.00	2.64
LYS44	HG3	1.00	0.019	1.00	2.94
LYS44	HD2	1.00	0.021	1.00	5.45
LYS44	HD3	1.00	0.021	1.00	5.45
LYS44	HE2	0.98	0.004	1.00	1.28
LYS44	H	1.00	0.003	1.00	-2953164.00
LEU45	H	1.00	0.010	1.00	-2947979.00
LEU45	HA	0.66	0.010	1.00	1.28

3.44.9 Detailed Probabilities of LYS44HB3:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS44	1.00	1.00
LEU45	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K44HA	1.00
K44HB2	1.00
K44HG2	1.00
K44HG3	1.00
K44HD2	1.00
K44HD3	1.00
K44HE2	0.99
K44H	1.00
K44HB3	1.00
L45H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS44	HA	1.00	0.006	1.00	3.96
LYS44	HB2	1.00	0.002	1.00	53.87
LYS44	HB3	1.00	0.002	1.00	53.87
LYS44	HG2	1.00	0.012	1.00	2.64
LYS44	HG3	1.00	0.014	1.00	2.94
LYS44	HD2	1.00	0.026	1.00	5.45
LYS44	HD3	1.00	0.026	1.00	5.45
LYS44	HE2	0.99	0.009	1.00	1.28
LYS44	H	1.00	0.002	1.00	-2953164.00
LEU45	H	1.00	0.005	1.00	-2947979.00
LEU45	HA	0.85	0.005	1.00	1.28

3.44.10 Detailed Probabilities of LYS44HG2:

Overall probability: 0.633

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS44	0.70	0.90
LEU45	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
K44HA	1.00
K44HB2	1.00
K44HB3	1.00
K44HG3	1.00
K44HD2	1.00
K44HD3	1.00
K44HE2	1.00
K44H	1.00
K44HZ2	1.00
K44HG2	1.00
L45H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS44	HA	1.00	0.037	0.30	0.00
LYS44	HB2	1.00	0.001	1.00	3.20
LYS44	HB3	1.00	0.001	1.00	3.20
LYS44	HG2	1.00	0.018	1.00	27.11
LYS44	HG3	1.00	0.010	1.00	8.71
LYS44	HD2	1.00	0.085	0.00	0.00
LYS44	HD3	1.00	0.085	0.00	0.00
LYS44	HE2	1.00	0.022	1.00	1.96
LYS44	H	1.00	0.004	1.00	-855885.00
LEU45	H	0.97	0.083	0.03	0.00

3.44.11 Detailed Probabilities of LYS44HG3:

Overall probability: 0.767

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS44	0.77	0.90

Expected NOESY Contacts

Proton	Expected probability
K44HA	1.00
K44HB2	1.00
K44HB3	1.00
K44HG2	1.00
K44HD2	1.00
K44HD3	1.00
K44HE2	1.00
K44H	1.00
K44HZ2	1.00
K44HG3	1.00

NOESY contacts detailed probability

3.44 LYS(44)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS44	HA	1.00	0.001	1.00	1.07
LYS44	HB2	1.00	0.035	0.50	0.00
LYS44	HB3	1.00	0.035	0.50	0.00
LYS44	HG2	1.00	0.021	1.00	7.46
LYS44	HG3	1.00	0.031	0.90	0.00
LYS44	HD2	1.00	0.035	0.50	0.00
LYS44	HD3	1.00	0.035	0.50	0.00
LYS44	HE2	1.00	0.027	1.00	1.85
LYS44	H	1.00	0.001	1.00	-383812.00

3.44.12 Detailed Probabilities of LYS44HD2:

Overall probability: 0.822

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS44	0.82	0.89

Expected NOESY Contacts

Proton	Expected probability
K44HA	0.98
K44HB2	1.00
K44HB3	1.00
K44HG2	1.00
K44HG3	1.00
K44HD3	1.00
K44HE2	1.00
K44HZ2	1.00
K44HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS44	HA	0.98	0.014	1.00	1.91
LYS44	HB2	1.00	0.017	1.00	5.56
LYS44	HB3	1.00	0.017	1.00	5.56
LYS44	HG2	1.00	0.075	0.00	0.00
LYS44	HG3	1.00	0.013	1.00	6.92
LYS44	HD2	1.00	0.016	1.00	244.35
LYS44	HD3	1.00	0.016	1.00	244.35
LYS44	HE2	1.00	0.036	0.40	0.00
LYS44	H	0.88	0.011	1.00	-421987.00

3.44.13 Detailed Probabilities of LYS44HD3:

Overall probability: 0.800

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS44	0.80	0.89

Expected NOESY Contacts

Proton	Expected probability
K44HA	0.98
K44HB2	1.00
K44HB3	1.00
K44HG2	1.00
K44HG3	1.00
K44HD2	1.00
K44HE2	1.00
K44HZ2	1.00
K44HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS44	HA	0.98	0.016	1.00	1.91
LYS44	HB2	1.00	0.019	1.00	5.56
LYS44	HB3	1.00	0.019	1.00	5.56
LYS44	HG2	1.00	0.077	0.00	0.00
LYS44	HG3	1.00	0.015	1.00	6.92
LYS44	HD2	1.00	0.018	1.00	244.35
LYS44	HD3	1.00	0.018	1.00	244.35
LYS44	HE2	1.00	0.038	0.20	0.00
LYS44	H	0.87	0.013	1.00	-421987.00

3.44.14 Detailed Probabilities of LYS44HE2:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS44	1.00	0.88

Expected NOESY Contacts

Proton	Expected probability
K44HB2	0.98
K44HB3	0.99
K44HG2	1.00
K44HG3	1.00
K44HD2	1.00
K44HD3	1.00
K44HE3	1.00
K44HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS44	HB2	0.99	0.001	1.00	0.70
LYS44	HB3	0.99	0.001	1.00	0.70
LYS44	HG2	1.00	0.003	1.00	1.05
LYS44	HG3	1.00	0.030	1.00	0.86
LYS44	HD2	1.00	0.017	1.00	4.26
LYS44	HD3	1.00	0.017	1.00	4.26
LYS44	HE2	1.00	0.013	1.00	220.78
LYS44	HA	0.76	0.007	1.00	0.40

3.44.15 Detailed Probabilities of LYS44H:

Overall probability: 0.621

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS43	0.35	1.00
LYS44	0.83	1.00
LEU45	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K43HB2	1.00
K43HG3	0.96
K43HB3	1.00
K43HA	1.00
K43HG2	0.97
K43H	1.00
K44HA	1.00
K44HB2	1.00
K44HB3	1.00
K44HG2	1.00
K44HG3	1.00
K44H	1.00
L45H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS43	HA	1.00	0.040	0.00	0.00
LYS43	HB2	1.00	0.028	1.00	1.72
LYS43	HB3	1.00	0.028	1.00	1.72
LYS43	HG2	0.97	0.055	0.03	0.00
LYS43	HG3	0.96	0.049	0.04	0.00
LYS43	H	1.00	0.055	0.00	0.00
LYS44	HA	1.00	0.040	0.00	0.00
LYS44	HB2	1.00	0.028	1.00	1.72
LYS44	HB3	1.00	0.028	1.00	1.72
LYS44	HG2	1.00	0.006	1.00	0.45
LYS44	HG3	1.00	0.010	1.00	0.23
LYS44	H	1.00	0.005	1.00	-10036825.00
LEU45	H	1.00	0.008	1.00	-887386.00

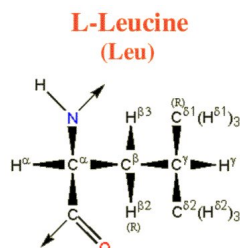
3.45 LEU(45)

Figure 44: Image from the BMRB

Residue probability: 0.897

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.357	177.056	1.929	0.000	0.000
CA 3.45.1	57.187	55.735	3.802	0.742	1.000
CB 3.45.2	41.773	42.389	3.750	1.000	1.000
CG 3.45.3	26.770	26.892	3.086	0.838	1.000
CD1 3.45.4	25.491	24.837	3.657	1.000	1.000
CD2 3.45.5	23.696	24.201	3.117	1.000	1.000
N 3.45.6	117.785	121.785	4.943	0.930	1.000
HA 3.45.7	4.148	4.315	0.840	0.500	1.000
HB2 3.45.8	1.904	1.601	0.373	0.967	1.000
HB3 3.45.9	1.486	1.508	0.398	0.875	1.000
HG 3.45.10	1.882	1.510	0.340	0.875	1.000
HD1 3.45.11	0.754	0.739	0.294	1.000	1.000
HD2 3.45.12	0.725	0.727	0.421	1.000	1.000
H 3.45.13	8.161	8.237	0.647	0.933	1.000

3.45.1 Detailed Probabilities of LEU45CA:

Overall probability: 0.742

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS44	0.67	1.00
LEU45	0.86	1.00
ALA46	0.45	1.00

Expected NOESY Contacts

Proton	Expected probability
K44HA	1.00
L45HB2	1.00
L45HB3	1.00
L45HG	1.00
L45HD11	0.99
L45HD21	0.99
L45H	1.00
L45HA	1.00
A46HA	1.00
A46H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS44	HA	1.00	0.122	0.00	0.00
LYS44	HB2	0.66	0.010	1.00	1.28
LYS44	HB3	0.85	0.005	1.00	1.28
LEU45	HA	1.00	0.209	0.00	0.00
LEU45	HB2	1.00	0.003	1.00	1.28
LEU45	HB3	1.00	0.006	1.00	0.85
LEU45	HG	1.00	0.019	1.00	1.28
LEU45	HD11	0.99	0.022	1.00	1.84
LEU45	HD21	0.99	0.007	1.00	1.84
LEU45	H	1.00	0.002	1.00	0.59
ALA46	HA	1.00	0.136	0.00	0.00
ALA46	H	1.00	0.031	0.90	0.00

3.45.2 Detailed Probabilities of LEU45CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU45	1.00	1.00
ALA46	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L45HA	1.00
L45HB2	1.00
L45HG	1.00
L45HD11	1.00
L45HD21	1.00
L45H	1.00
L45HB3	1.00
A46H	1.00

NOESY contacts detailed probability

3.45 LEU(45)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU45	HA	1.00	0.001	1.00	0.54
LEU45	HB2	1.00	0.001	1.00	2.48
LEU45	HB3	1.00	0.019	1.00	4.01
LEU45	HG	1.00	0.021	1.00	2.48
LEU45	HD11	1.00	0.005	1.00	1.16
LEU45	HD21	1.00	0.024	1.00	1.16
LEU45	H	1.00	0.004	1.00	0.44
ALA46	H	1.00	0.005	1.00	0.30
ALA46	HA	0.92	0.014	1.00	0.18

3.45.3 Detailed Probabilities of LEU45CG:

Overall probability: 0.838

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU45	0.81	1.00
ALA46	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L45HA	1.00
L45HB2	1.00
L45HB3	1.00
L45HD11	1.00
L45HD21	1.00
L45H	1.00
L45HG	1.00
A46H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU45	HA	1.00	0.072	0.00	0.00
LEU45	HB2	1.00	0.033	0.70	0.00
LEU45	HB3	1.00	0.014	1.00	0.46
LEU45	HG	1.00	0.011	1.00	12.24
LEU45	HD11	1.00	0.019	1.00	1.09
LEU45	HD21	1.00	0.010	1.00	1.09
LEU45	H	1.00	0.003	1.00	0.64
ALA46	H	0.98	0.011	1.00	0.14

3.45.4 Detailed Probabilities of LEU45CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU45	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L45HA	0.99
L45HB2	1.00
L45HB3	1.00
L45HG	1.00
L45HD12	1.00
L45HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU45	HA	0.99	0.008	1.00	0.35
LEU45	HB2	1.00	0.016	1.00	2.66
LEU45	HB3	1.00	0.026	1.00	3.61
LEU45	HG	1.00	0.006	1.00	2.66
LEU45	HD11	1.00	0.001	1.00	119.01
LEU45	HD21	1.00	0.002	1.00	164.25

3.45.5 Detailed Probabilities of LEU45CD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU45	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L45HA	0.99
L45HB2	1.00
L45HB3	1.00
L45HG	1.00
L45HD11	1.00
L45HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU45	HA	0.99	0.000	1.00	1.40
LEU45	HB2	1.00	0.009	1.00	1.87
LEU45	HB3	1.00	0.008	1.00	1.01
LEU45	HG	1.00	0.013	1.00	1.87
LEU45	HD11	1.00	0.024	1.00	51.95
LEU45	HD21	1.00	0.005	1.00	51.95

3.45.6 Detailed Probabilities of LEU45N:

Overall probability: 0.930

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS44	0.81	1.00
LEU45	1.00	1.00
ALA46	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K44HB3	1.00
K44HG2	0.97
K44H	1.00
K44HB2	1.00
K44HA	1.00
L45HA	1.00
L45HB2	1.00
L45HB3	1.00
L45HG	1.00
L45H	1.00
A46H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS44	HA	1.00	0.003	1.00	-320505.00
LYS44	HB2	1.00	0.010	1.00	-2947979.00
LYS44	HB3	1.00	0.005	1.00	-2947979.00
LYS44	HG2	0.97	0.083	0.03	0.00
LYS44	H	1.00	0.008	1.00	-887386.00
LEU45	HA	1.00	0.002	1.00	-624113.00
LEU45	HB2	1.00	0.003	1.00	-2947979.00
LEU45	HB3	1.00	0.013	1.00	-600443.00
LEU45	HG	1.00	0.019	1.00	-2947979.00
LEU45	H	1.00	0.003	1.00	-7553914.00
LEU45	HD11	0.88	0.013	1.00	-695524.00
LEU45	HD21	0.87	0.016	1.00	-695524.00
ALA46	H	1.00	0.006	1.00	-888177.00
ALA46	HA	0.90	0.010	1.00	-197707.00

3.45.7 Detailed Probabilities of LEU45HA:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS44	0.00	1.00
LEU45	0.71	1.00
ALA46	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K44HA	1.00
L45HB2	1.00
L45HB3	1.00
L45HG	1.00
L45HD11	0.99
L45HD21	0.99
L45H	1.00
L45HA	1.00
A46HA	1.00
A46H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS44	HA	1.00	0.106	0.00	0.00
LEU45	HA	1.00	0.209	0.00	0.00
LEU45	HB2	1.00	0.012	1.00	0.74
LEU45	HB3	1.00	0.001	1.00	0.54
LEU45	HG	1.00	0.072	0.00	0.00
LEU45	HD11	0.99	0.008	1.00	0.35
LEU45	HD21	0.99	0.000	1.00	1.40
LEU45	H	1.00	0.002	1.00	-624113.00
ALA46	HA	1.00	0.108	0.00	0.00
ALA46	H	1.00	0.081	0.00	0.00

3.45.8 Detailed Probabilities of LEU45HB2:

Overall probability: 0.967

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU45	0.96	1.00
ALA46	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L45HA	1.00
L45HB3	1.00
L45HG	1.00
L45HD11	1.00
L45HD21	1.00
L45H	1.00
L45HB2	1.00
A46H	1.00

NOESY contacts detailed probability

3.45 LEU(45)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU45	HA	1.00	0.003	1.00	1.28
LEU45	HB2	1.00	0.022	1.00	5.90
LEU45	HB3	1.00	0.001	1.00	2.48
LEU45	HG	1.00	0.033	0.70	0.00
LEU45	HD11	1.00	0.016	1.00	2.66
LEU45	HD21	1.00	0.009	1.00	1.87
LEU45	H	1.00	0.003	1.00	-2947979.00
ALA46	H	1.00	0.002	1.00	-1317662.00
ALA46	HA	0.66	0.010	1.00	0.12

3.45.9 Detailed Probabilities of LEU45HB3:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU45	1.00	1.00
ALA46	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L45HA	1.00
L45HB2	1.00
L45HG	1.00
L45HD11	1.00
L45HD21	1.00
L45H	1.00
L45HB3	1.00
A46H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU45	HA	1.00	0.006	1.00	0.85
LEU45	HB2	1.00	0.012	1.00	1.99
LEU45	HB3	1.00	0.019	1.00	4.01
LEU45	HG	1.00	0.014	1.00	0.46
LEU45	HD11	1.00	0.026	1.00	3.61
LEU45	HD21	1.00	0.008	1.00	1.01
LEU45	H	1.00	0.013	1.00	-600443.00
ALA46	H	1.00	0.062	0.00	0.00

3.45.10 Detailed Probabilities of LEU45HG:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU45	0.86	1.00
ALA46	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L45HA	1.00
L45HB2	1.00
L45HB3	1.00
L45HD11	1.00
L45HD21	1.00
L45H	1.00
L45HG	1.00
A46H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU45	HA	1.00	0.019	1.00	1.28
LEU45	HB2	1.00	0.044	0.00	0.00
LEU45	HB3	1.00	0.021	1.00	2.48
LEU45	HG	1.00	0.011	1.00	12.24
LEU45	HD11	1.00	0.006	1.00	2.66
LEU45	HD21	1.00	0.013	1.00	1.87
LEU45	H	1.00	0.019	1.00	-2947979.00
ALA46	H	0.98	0.020	1.00	-1317662.00

3.45.11 Detailed Probabilities of LEU45HD11:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU45	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L45HA	0.99
L45HB2	1.00
L45HB3	1.00
L45HG	1.00
L45HD12	1.00
L45HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU45	HA	0.99	0.022	1.00	1.84
LEU45	HB2	1.00	0.006	1.00	0.85
LEU45	HB3	1.00	0.005	1.00	1.16
LEU45	HG	1.00	0.019	1.00	1.09
LEU45	HD11	1.00	0.001	1.00	119.01
LEU45	HD21	1.00	0.024	1.00	51.95
LEU45	H	0.86	0.013	1.00	-695524.00

3.45.12 Detailed Probabilities of LEU45HD21:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU45	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L45HA	0.99
L45HB2	1.00
L45HB3	1.00
L45HG	1.00
L45HD11	1.00
L45HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU45	HA	0.99	0.007	1.00	1.84
LEU45	HB2	1.00	0.023	1.00	0.85
LEU45	HB3	1.00	0.024	1.00	1.16
LEU45	HG	1.00	0.010	1.00	1.09
LEU45	HD11	1.00	0.002	1.00	164.25
LEU45	HD21	1.00	0.005	1.00	51.95
LEU45	H	0.85	0.016	1.00	-695524.00

3.45.13 Detailed Probabilities of LEU45H:

Overall probability: 0.933

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS44	0.88	1.00
LEU45	1.00	1.00
ALA46	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K44HB3	1.00
K44HG2	0.97
K44H	1.00
K44HB2	1.00
K44HA	1.00
L45HA	1.00
L45HB2	1.00
L45HB3	1.00
L45HG	1.00
L45H	1.00
A46H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS44	HA	1.00	0.069	0.00	0.00
LYS44	HB2	1.00	0.001	1.00	0.64
LYS44	HB3	1.00	0.001	1.00	0.64
LYS44	HG2	0.97	0.001	1.00	0.10
LYS44	H	1.00	0.003	1.00	-961380.00
LYS44	HG3	0.95	0.005	1.00	0.08
LYS44	HD2	0.54	0.001	1.00	0.12
LYS44	HD3	0.56	0.001	1.00	0.12
LEU45	HA	1.00	0.002	1.00	0.59
LEU45	HB2	1.00	0.003	1.00	0.52
LEU45	HB3	1.00	0.004	1.00	0.44
LEU45	HG	1.00	0.003	1.00	0.64
LEU45	H	1.00	0.003	1.00	-7553914.00
ALA46	H	1.00	0.004	1.00	-948656.00
ALA46	HA	0.90	0.000	1.00	0.05

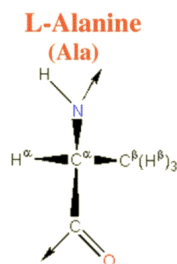
3.46 ALA(46)

Figure 45: Image from the BMRB

Residue probability: 0.841

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	53.672	53.289	3.425	0.750	1.000
CB 3.46.2	18.882	19.355	4.103	0.800	1.000
N 3.46.3	118.538	123.100	4.487	0.750	1.000
HA 3.46.4	4.252	4.254	0.459	0.856	1.000
HB 3.46.5	1.550	1.346	0.258	1.000	1.000
H 3.46.6	7.637	8.206	0.601	0.890	1.000

3.46.1 Detailed Probabilities of ALA46CA:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU45	0.67	1.00
ALA46	1.00	1.00
GLU47	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
L45HA	1.00
A46H	1.00
A46HB1	1.00
A46HA	1.00
E47H	1.00
E47HA	1.00

NOESY contacts detailed probability

3.46 ALA(46)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU45	HA	1.00	0.108	0.00	0.00
LEU45	HB2	0.66	0.010	1.00	0.12
LEU45	H	0.90	0.000	1.00	0.05
ALA46	HA	1.00	0.004	1.00	8.19
ALA46	HB1	1.00	0.000	1.00	2.33
ALA46	H	1.00	0.010	1.00	0.60
GLU47	HA	1.00	0.006	1.00	8.19
GLU47	H	1.00	0.066	0.00	0.00

3.46.2 Detailed Probabilities of ALA46CB:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ALA46	1.00	1.00
GLU47	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
A46HA	1.00
A46H	1.00
A46HB2	1.00
E47H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA46	HA	1.00	0.004	1.00	3.41
ALA46	HB1	1.00	0.001	1.00	58.56
ALA46	H	1.00	0.008	1.00	2.50
GLU47	H	1.00	0.068	0.00	0.00
GLU47	HA	0.71	0.006	1.00	3.41

3.46.3 Detailed Probabilities of ALA46N:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU45	0.60	1.00
ALA46	1.00	1.00
GLU47	0.75	1.00

Expected NOESY Contacts

Proton	Expected probability
L45HG	0.98
L45HB3	1.00
L45H	1.00
L45HA	1.00
L45HB2	1.00
A46HA	1.00
A46HB1	1.00
A46H	1.00
E47H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU45	HA	1.00	0.081	0.00	0.00
LEU45	HB2	1.00	0.002	1.00	-1317662.00
LEU45	HB3	1.00	0.062	0.00	0.00
LEU45	HG	0.98	0.020	1.00	-1317662.00
LEU45	H	1.00	0.004	1.00	-948656.00
ALA46	HA	1.00	0.004	1.00	-1150780.00
ALA46	HB1	1.00	0.002	1.00	-3332692.00
ALA46	H	1.00	0.007	1.00	-19107776.00
GLU47	H	1.00	0.035	0.50	0.00
GLU47	HA	0.89	0.006	1.00	-1150780.00

3.46.4 Detailed Probabilities of ALA46HA:

Overall probability: 0.856

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU45	0.67	1.00
ALA46	1.00	1.00
GLU47	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L45HA	1.00
A46H	1.00
A46HB1	1.00
A46HA	1.00
E47H	1.00
E47HA	1.00

NOESY contacts detailed probability

3.46 ALA(46)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU45	HA	1.00	0.136	0.00	0.00
LEU45	HB2	0.66	0.033	0.70	0.00
LEU45	HB3	0.92	0.014	1.00	0.18
LEU45	H	0.90	0.010	1.00	-197707.00
ALA46	HA	1.00	0.004	1.00	8.19
ALA46	HB1	1.00	0.004	1.00	3.41
ALA46	H	1.00	0.004	1.00	-1150780.00
GLU47	HA	1.00	0.006	1.00	14.88
GLU47	H	1.00	0.002	1.00	-1032311.00

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
GLU47	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
A46HA	1.00
A46H	1.00
A46HB2	1.00
E47H	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	2.33
ALA46	HB1	1.00	0.001	1.00	58.56
ALA46	H	1.00	0.002	1.00	-3332692.00
GLU47	H	1.00	0.002	1.00	-937692.00

3.46.6 Detailed Probabilities of ALA46H:

Overall probability: 0.890

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU45	0.98	1.00
ALA46	1.00	1.00
GLU47	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L45HG	0.98
L45HB3	1.00
L45H	1.00
L45HA	1.00
L45HB2	1.00
A46HA	1.00
A46HB1	1.00
A46H	1.00
E47H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU45	HA	1.00	0.031	0.90	0.00
LEU45	HB2	1.00	0.013	1.00	0.29
LEU45	HB3	1.00	0.005	1.00	0.30
LEU45	HG	0.98	0.011	1.00	0.14
LEU45	H	1.00	0.006	1.00	-888177.00
LEU45	HD11	0.53	0.004	1.00	0.45
ALA46	HA	1.00	0.010	1.00	0.60
ALA46	HB1	1.00	0.008	1.00	2.50
ALA46	H	1.00	0.007	1.00	-19107776.00
GLU47	H	1.00	0.082	0.00	0.00

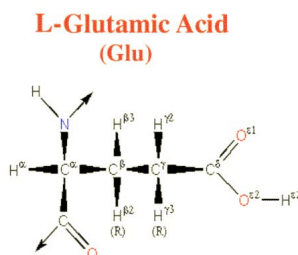


Figure 46: Image from the BMRB

Residue probability: 0.654
Residue probability confidence: 0.925

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	176.478	176.942	2.547	0.000	0.000
CA 3.47.1	56.931	57.442	3.837	0.556	1.000
CB 3.47.2	30.417	30.185	4.018	0.571	0.875
CG 3.47.3	36.271	36.085	1.533	1.000	0.875
N 3.47.4	115.492	120.574	4.837	0.833	1.000
HA 3.47.5	4.250	4.245	0.429	0.818	1.000
HB2 3.47.6	2.056	2.021	0.233	0.429	0.875
HB3 3.47.7	2.110	1.994	0.244	0.250	0.875
HG2 3.47.8	2.295	2.258	0.226	0.714	0.875
HG3 3.47.9	2.500	2.233	0.232	0.719	0.875
H 3.47.10	7.713	8.332	0.601	0.650	1.000
HE2	NA	—	—	0.000	0.000

3.47.1 Detailed Probabilities of GLU47CA:

Overall probability: 0.556
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ALA46	1.00	1.00
GLU47	0.50	1.00
GLU48	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
A46HA	1.00
E47HB2	1.00
E47HB3	1.00
E47HG2	1.00
E47HG3	1.00
E47H	1.00
E47HA	1.00
E48H	1.00
E48HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA46	HA	1.00	0.006	1.00	14.88
GLU47	HA	1.00	0.004	1.00	14.88
GLU47	HB2	1.00	0.234	0.00	0.00
GLU47	HB3	1.00	0.180	0.00	0.00
GLU47	HG2	1.00	0.005	1.00	0.93
GLU47	HG3	1.00	0.210	0.00	0.00
GLU47	H	1.00	0.015	1.00	0.93
GLU48	HA	1.00	0.119	0.00	0.00
GLU48	H	1.00	0.020	1.00	0.93

3.47.2 Detailed Probabilities of GLU47CB:

Overall probability: 0.571

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU47	0.50	0.86
GLU48	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E47HA	1.00
E47HB3	1.00
E47HG2	1.00
E47HG3	1.00
E47H	1.00
E47HE2	1.00
E47HB2	1.00
E48H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU47	HA	1.00	0.001	1.00	0.84
GLU47	HB2	1.00	0.443	0.00	0.00
GLU47	HB3	1.00	0.389	0.00	0.00
GLU47	HG2	1.00	0.204	0.00	0.00
GLU47	HG3	1.00	0.001	1.00	0.50
GLU47	H	1.00	0.011	1.00	0.59
GLU48	H	1.00	0.024	1.00	0.59

3.47.3 Detailed Probabilities of GLU47CG:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU47	1.00	0.86
GLU48	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E47HA	1.00
E47HB2	1.00
E47HB3	1.00
E47HG3	1.00
E47H	1.00
E47HE2	1.00
E47HG2	1.00
E48H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU47	HA	1.00	0.001	1.00	1.06
GLU47	HB2	1.00	0.024	1.00	8.87
GLU47	HB3	1.00	0.030	1.00	8.87
GLU47	HG2	1.00	0.001	1.00	100.68
GLU47	HG3	1.00	0.004	1.00	5.64
GLU47	H	1.00	0.028	1.00	0.20
GLU48	H	0.98	0.007	1.00	0.20

3.47.4 Detailed Probabilities of GLU47N:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ALA46	0.67	1.00
GLU47	0.83	1.00
GLU48	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
A46HB1	1.00
A46HA	1.00
A46H	1.00
E47HA	1.00
E47HB2	1.00
E47HB3	1.00
E47HG2	1.00
E47HG3	1.00
E47H	1.00
E48H	1.00

NOESY contacts detailed probability

3.47 GLU(47)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA46	HA	1.00	0.002	1.00	-1032311.00
ALA46	HB1	1.00	0.002	1.00	-937692.00
ALA46	H	1.00	0.082	0.00	0.00
GLU47	HA	1.00	0.000	1.00	-1032311.00
GLU47	HB2	1.00	0.010	1.00	-1144478.00
GLU47	HB3	1.00	0.044	0.00	0.00
GLU47	HG2	1.00	0.003	1.00	-424775.00
GLU47	HG3	1.00	0.001	1.00	-642559.00
GLU47	H	1.00	0.006	1.00	-8340350.00
GLU48	H	1.00	0.029	1.00	-8340350.00
GLU48	HA	0.88	0.020	1.00	-86617.00
GLU48	HB2	0.67	0.026	1.00	-1144478.00

3.47.5 Detailed Probabilities of GLU47HA:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ALA46	1.00	1.00
GLU47	1.00	1.00
GLU48	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
A46HA	1.00
E47HB2	1.00
E47HB3	1.00
E47HG2	1.00
E47HG3	1.00
E47H	1.00
E47HA	1.00
E48H	1.00
E48HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA46	HA	1.00	0.006	1.00	8.19
ALA46	HB1	0.66	0.006	1.00	3.41
ALA46	H	0.89	0.006	1.00	-1150780.00
GLU47	HA	1.00	0.004	1.00	14.88
GLU47	HB2	1.00	0.001	1.00	0.84
GLU47	HB3	1.00	0.001	1.00	0.79
GLU47	HG2	1.00	0.001	1.00	1.06
GLU47	HG3	1.00	0.000	1.00	0.57
GLU47	H	1.00	0.000	1.00	-1032311.00
GLU48	HA	1.00	0.253	0.00	0.00
GLU48	H	1.00	0.055	0.00	0.00

3.47.6 Detailed Probabilities of GLU47HB2:

Overall probability: 0.429

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU47	0.33	0.86
GLU48	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E47HA	1.00
E47HB3	1.00
E47HG2	1.00
E47HG3	1.00
E47H	1.00
E47HE2	1.00
E47HB2	1.00
E48H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU47	HA	1.00	0.234	0.00	0.00
GLU47	HB2	1.00	0.443	0.00	0.00
GLU47	HB3	1.00	0.440	0.00	0.00
GLU47	HG2	1.00	0.024	1.00	8.87
GLU47	HG3	1.00	0.125	0.00	0.00
GLU47	H	1.00	0.010	1.00	-1144478.00
GLU48	H	1.00	0.029	1.00	-719654.00

3.47.7 Detailed Probabilities of GLU47HB3:

Overall probability: 0.250

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU47	0.17	0.86
GLU48	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E47HA	1.00
E47HB2	1.00
E47HG2	1.00
E47HG3	1.00
E47H	1.00
E47HE2	1.00
E47HB3	1.00
E48H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU47	HA	1.00	0.180	0.00	0.00
GLU47	HB2	1.00	0.389	0.00	0.00
GLU47	HB3	1.00	0.386	0.00	0.00
GLU47	HG2	1.00	0.030	1.00	8.87
GLU47	HG3	1.00	0.179	0.00	0.00
GLU47	H	1.00	0.044	0.00	0.00
GLU48	H	1.00	0.083	0.00	0.00
GLU48	HA	0.81	0.019	1.00	0.52

3.47.8 Detailed Probabilities of GLU47HG2:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU47	0.67	0.86
GLU48	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E47HA	1.00
E47HB2	1.00
E47HB3	1.00
E47HG3	1.00
E47H	1.00
E47HE2	1.00
E47HG2	1.00
E48H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU47	HA	1.00	0.005	1.00	0.93
GLU47	HB2	1.00	0.204	0.00	0.00
GLU47	HB3	1.00	0.201	0.00	0.00
GLU47	HG2	1.00	0.001	1.00	100.68
GLU47	HG3	1.00	0.002	1.00	6.01
GLU47	H	1.00	0.003	1.00	-424775.00
GLU48	H	0.98	0.030	1.00	0.00

3.47.9 Detailed Probabilities of GLU47HG3:

Overall probability: 0.719

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU47	0.83	0.86
GLU48	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
E47HA	1.00
E47HB2	1.00
E47HB3	1.00
E47HG2	1.00
E47H	1.00
E47HE2	1.00
E47HG3	1.00
E48H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU47	HA	1.00	0.210	0.00	0.00
GLU47	HB2	1.00	0.001	1.00	0.50
GLU47	HB3	1.00	0.004	1.00	0.61
GLU47	HG2	1.00	0.004	1.00	5.64
GLU47	HG3	1.00	0.003	1.00	13.85
GLU47	H	1.00	0.001	1.00	-642559.00
GLU48	H	0.97	0.175	0.03	0.00

3.47.10 Detailed Probabilities of GLU47H:

Overall probability: 0.650

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ALA46	0.17	1.00
GLU47	0.83	1.00
GLU48	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
A46HB1	1.00
A46HA	1.00
A46H	1.00
E47HA	1.00
E47HB2	1.00
E47HB3	1.00
E47HG2	1.00
E47HG3	1.00
E47H	1.00
E48H	1.00

NOESY contacts detailed probability

3.47 GLU(47)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA46	HA	1.00	0.066	0.00	0.00
ALA46	HB1	1.00	0.068	0.00	0.00
ALA46	H	1.00	0.035	0.50	0.00
GLU47	HA	1.00	0.015	1.00	0.93
GLU47	HB2	1.00	0.011	1.00	0.59
GLU47	HB3	1.00	0.621	0.00	0.00
GLU47	HG2	1.00	0.028	1.00	0.20
GLU47	HG3	1.00	0.007	1.00	0.61
GLU47	H	1.00	0.006	1.00	-8340350.00
GLU48	H	1.00	0.012	1.00	-6784282.00

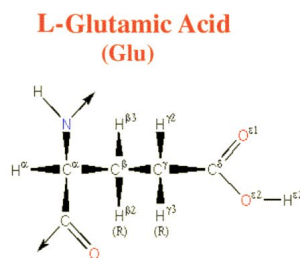


Figure 47: Image from the BMRB

Residue probability: 0.538
Residue probability confidence: 0.921

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	173.624	176.942	2.547	0.000	0.000
CA 3.48.1	56.021	57.442	3.837	0.444	1.000
CB 3.48.2	29.910	30.185	4.018	0.743	0.857
CG 3.48.3	36.010	36.085	1.533	0.517	0.857
N 3.48.4	120.573	120.574	4.837	0.645	1.000
HA 3.48.5	4.373	4.245	0.429	0.389	1.000
HB 3.48.6	2.040	2.021	0.233	0.429	0.857
HG2 3.48.7	2.202	2.258	0.226	0.337	0.857
HG3 3.48.8	2.319	2.233	0.232	0.673	0.857
H 3.48.9	7.748	8.332	0.601	0.667	1.000
HE2	NA	—	—	0.000	0.000

3.48.1 Detailed Probabilities of GLU48CA:

Overall probability: 0.444
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU47	0.50	1.00
GLU48	0.40	1.00
LYS49	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E47HA	1.00
E48HB2	1.00
E48HG2	1.00
E48HG3	1.00
E48H	1.00
E48HA	1.00
K49HA	1.00
K49H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU47	HA	1.00	0.253	0.00	0.00
GLU47	HB3	0.81	0.019	1.00	0.52
GLU48	HA	1.00	0.243	0.00	0.00
GLU48	HB2	1.00	0.089	0.00	0.00
GLU48	HG2	1.00	0.073	0.00	0.00
GLU48	HG3	1.00	0.017	1.00	0.39
GLU48	H	1.00	0.004	1.00	0.38
LYS49	HA	1.00	0.298	0.00	0.00
LYS49	H	1.00	0.005	1.00	0.54

3.48.2 Detailed Probabilities of GLU48CB:

Overall probability: 0.743

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU48	0.70	0.83
LYS49	0.85	1.00

Expected NOESY Contacts

Proton	Expected probability
E48HA	1.00
E48HB3	1.00
E48HG2	1.00
E48HG3	1.00
E48H	1.00
E48HE2	1.00
K49H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU48	HA	1.00	0.035	0.50	0.00
GLU48	HB2	1.00	0.001	1.00	52.03
GLU48	HG2	1.00	0.020	1.00	14.03
GLU48	HG3	1.00	0.016	1.00	4.32
GLU48	H	1.00	0.060	0.00	0.00
LYS49	H	1.00	0.033	0.70	0.00
LYS49	HA	0.79	0.020	1.00	2.30

3.48.3 Detailed Probabilities of GLU48CG:

Overall probability: 0.517

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU48	0.60	0.83
LYS49	0.10	1.00

Expected NOESY Contacts

Proton	Expected probability
E48HA	1.00
E48HB2	1.00
E48HG2	1.00
E48H	1.00
E48HE2	1.00
E48HG3	1.00
K49H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU48	HA	1.00	0.006	1.00	0.22
GLU48	HB2	1.00	0.040	0.00	0.00
GLU48	HG2	1.00	0.122	0.00	0.00
GLU48	HG3	1.00	0.023	1.00	100.68
GLU48	H	1.00	0.007	1.00	0.20
LYS49	H	0.96	0.039	0.10	0.00

3.48.4 Detailed Probabilities of GLU48N:

Overall probability: 0.645

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU47	0.50	1.00
GLU48	0.60	1.00
LYS49	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E47HG2	0.98
E47HA	1.00
E47H	1.00
E47HB3	1.00
E47HG3	0.97
E47HB2	1.00
E48HA	1.00
E48HB2	1.00
E48HG2	1.00
E48HG3	1.00
E48H	1.00
K49H	1.00

NOESY contacts detailed probability

3.48 GLU(48)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU47	HA	1.00	0.055	0.00	0.00
GLU47	HB2	1.00	0.029	1.00	-719654.00
GLU47	HB3	1.00	0.083	0.00	0.00
GLU47	HG2	0.98	0.030	1.00	0.00
GLU47	HG3	0.97	0.175	0.03	0.00
GLU47	H	1.00	0.012	1.00	-6784282.00
GLU48	HA	1.00	0.068	0.00	0.00
GLU48	HB2	1.00	0.013	1.00	-719654.00
GLU48	HG2	1.00	0.123	0.00	0.00
GLU48	HG3	1.00	0.006	1.00	-144808.00
GLU48	H	1.00	0.023	1.00	-6784282.00
LYS49	H	1.00	0.005	1.00	-121353.00
LYS49	HA	0.88	0.013	1.00	-830971.00
LYS49	HB2	0.62	0.018	1.00	-1133081.00

3.48.5 Detailed Probabilities of GLU48HA:

Overall probability: 0.389

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU47	0.50	1.00
GLU48	0.30	1.00
LYS49	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E47HA	1.00
E48HB2	1.00
E48HG2	1.00
E48HG3	1.00
E48H	1.00
E48HA	1.00
K49HA	1.00
K49H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU47	HA	1.00	0.119	0.00	0.00
GLU47	H	0.88	0.020	1.00	-86617.00
GLU48	HA	1.00	0.243	0.00	0.00
GLU48	HB2	1.00	0.035	0.50	0.00
GLU48	HG2	1.00	0.318	0.00	0.00
GLU48	HG3	1.00	0.006	1.00	0.22
GLU48	H	1.00	0.068	0.00	0.00
LYS49	HA	1.00	0.063	0.00	0.00
LYS49	H	1.00	0.009	1.00	-448858.00

3.48.6 Detailed Probabilities of GLU48HB2:

Overall probability: 0.429

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU48	0.40	0.83
LYS49	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E48HA	1.00
E48HB3	1.00
E48HG2	1.00
E48HG3	1.00
E48H	1.00
E48HE2	1.00
K49H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU48	HA	1.00	0.089	0.00	0.00
GLU48	HB2	1.00	0.001	1.00	52.03
GLU48	HG2	1.00	0.139	0.00	0.00
GLU48	HG3	1.00	0.040	0.00	0.00
GLU48	H	1.00	0.013	1.00	-719654.00
LYS49	H	1.00	0.134	0.00	0.00
LYS49	HA	0.79	0.000	1.00	1.02

3.48.7 Detailed Probabilities of GLU48HG2:

Overall probability: 0.337

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU48	0.40	0.83
LYS49	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
E48HA	1.00
E48HB2	1.00
E48HG3	1.00
E48H	1.00
E48HE2	1.00
E48HG2	1.00
K49H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU48	HA	1.00	0.073	0.00	0.00
GLU48	HB2	1.00	0.020	1.00	14.03
GLU48	HG2	1.00	0.009	1.00	21.87
GLU48	HG3	1.00	0.122	0.00	0.00
GLU48	H	1.00	0.123	0.00	0.00
LYS49	H	0.98	0.296	0.02	0.00

3.48.8 Detailed Probabilities of GLU48HG3:

Overall probability: 0.673

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU48	0.80	0.83
LYS49	0.04	1.00

Expected NOESY Contacts

Proton	Expected probability
E48HA	1.00
E48HB2	1.00
E48HG2	1.00
E48H	1.00
E48HE2	1.00
E48HG3	1.00
K49H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU48	HA	1.00	0.017	1.00	0.39
GLU48	HB2	1.00	0.016	1.00	4.32
GLU48	HG2	1.00	0.074	0.00	0.00
GLU48	HG3	1.00	0.023	1.00	100.68
GLU48	H	1.00	0.006	1.00	-144808.00
LYS49	H	0.96	0.413	0.04	0.00

3.48.9 Detailed Probabilities of GLU48H:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU47	0.83	1.00
GLU48	0.60	1.00
LYS49	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E47HG2	0.98
E47HA	1.00
E47H	1.00
E47HB3	1.00
E47HG3	0.97
E47HB2	1.00
E48HA	1.00
E48HB2	1.00
E48HG2	1.00
E48HG3	1.00
E48H	1.00
K49H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU47	HA	1.00	0.020	1.00	0.93
GLU47	HB2	1.00	0.024	1.00	0.59
GLU47	HB3	1.00	0.586	0.00	0.00
GLU47	HG2	0.98	0.007	1.00	0.20
GLU47	HG3	0.97	0.028	1.00	0.61
GLU47	H	1.00	0.029	1.00	-8340350.00
GLU48	HA	1.00	0.004	1.00	0.38
GLU48	HB2	1.00	0.060	0.00	0.00
GLU48	HG2	1.00	0.066	0.00	0.00
GLU48	HG3	1.00	0.007	1.00	0.20
GLU48	H	1.00	0.023	1.00	-6784282.00
LYS49	H	1.00	0.627	0.00	0.00

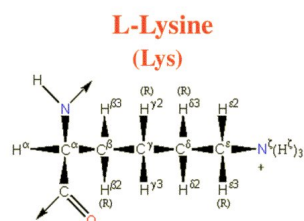


Figure 48: Image from the BMRB

Residue probability: 0.647
 Residue probability confidence: 0.935

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	176.843	176.660	3.133	0.000	0.000
CA 3.49.1	56.517	57.014	3.028	0.602	1.000
CB 3.49.2	32.462	32.981	3.186	0.875	1.000
CG 3.49.3	24.653	24.941	1.956	0.825	0.889
CD 3.49.4	28.780	29.020	2.193	0.529	0.857
CE 3.49.5	41.780	41.893	1.492	0.652	0.833
N 3.49.6	124.420	120.954	4.210	0.396	1.000
NZ	NA	—	—	0.000	0.000
HA 3.49.7	4.318	4.262	0.489	0.667	1.000
HB2 3.49.8	1.899	1.774	0.365	0.878	1.000
HB3 3.49.9	1.755	1.742	0.385	0.512	1.000
HG 3.49.10	1.458	1.358	0.344	0.644	0.889
HD 3.49.11	1.653	1.614	0.957	0.560	0.857
HE 3.49.12	3.015	2.907	0.230	0.543	0.833
H 3.49.13	8.607	8.185	0.605	0.735	1.000
HZ	NA	—	—	0.000	0.000

3.49.1 Detailed Probabilities of LYS49CA:

Overall probability: 0.602
 Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU48	0.50	1.00
LYS49	0.67	1.00
ASN50	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E48HA	1.00
K49HB2	1.00
K49HB3	1.00
K49HG2	1.00
K49HD2	0.98
K49H	1.00
K49HA	1.00
N50H	1.00
N50HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU48	HA	1.00	0.063	0.00	0.00
GLU48	HB2	0.64	0.000	1.00	1.02
LYS49	HA	1.00	0.008	1.00	21.81
LYS49	HB2	1.00	0.002	1.00	1.31
LYS49	HB3	1.00	0.010	1.00	0.70
LYS49	HG2	1.00	0.207	0.00	0.00
LYS49	HD2	0.98	0.112	0.02	0.00
LYS49	H	1.00	0.023	1.00	0.57
ASN50	HA	1.00	0.013	1.00	0.12
ASN50	H	1.00	0.093	0.00	0.00

3.49.2 Detailed Probabilities of LYS49CB:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS49	0.86	1.00
ASN50	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K49HA	1.00
K49HB2	1.00
K49HG2	1.00
K49HD2	1.00
K49HE2	0.99
K49H	1.00
K49HB3	1.00
N50H	1.00

NOESY contacts detailed probability

3.49 LYS(49)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS49	HA	1.00	0.001	1.00	0.61
LYS49	HB2	1.00	0.019	1.00	4.54
LYS49	HB3	1.00	0.013	1.00	9.08
LYS49	HG2	1.00	0.009	1.00	1.38
LYS49	HD2	1.00	0.115	0.00	0.00
LYS49	HE2	0.99	0.008	1.00	0.12
LYS49	H	1.00	0.000	1.00	0.57
ASN50	H	1.00	0.003	1.00	0.07

3.49.3 Detailed Probabilities of LYS49CG:

Overall probability: 0.825

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS49	0.80	0.88
ASN50	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K49HA	1.00
K49HB2	1.00
K49HB3	1.00
K49HG3	1.00
K49HD2	1.00
K49HE2	1.00
K49H	1.00
K49HZ2	1.00
N50H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS49	HA	1.00	0.003	1.00	0.81
LYS49	HB2	1.00	0.007	1.00	2.94
LYS49	HB3	1.00	0.034	0.60	0.00
LYS49	HG2	1.00	0.011	1.00	52.13
LYS49	HD2	1.00	0.029	1.00	6.34
LYS49	HE2	1.00	0.055	0.00	0.00
LYS49	H	1.00	0.005	1.00	0.22
ASN50	H	0.95	0.003	1.00	0.07

3.49.4 Detailed Probabilities of LYS49CD:

Overall probability: 0.529

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS49	0.53	0.86

Expected NOESY Contacts

Proton	Expected probability
K49HA	0.98
K49HB2	1.00
K49HB3	1.00
K49HG2	1.00
K49HD3	1.00
K49HE2	1.00
K49HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS49	HA	0.98	0.007	1.00	1.05
LYS49	HB2	1.00	0.215	0.00	0.00
LYS49	HB3	1.00	0.071	0.00	0.00
LYS49	HG2	1.00	0.039	0.10	0.00
LYS49	HD2	1.00	0.031	0.90	0.00
LYS49	HE2	1.00	0.033	0.70	0.00
LYS49	H	0.87	0.003	1.00	0.26

3.49.5 Detailed Probabilities of LYS49CE:

Overall probability: 0.652

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS49	0.65	0.83

Expected NOESY Contacts

Proton	Expected probability
K49HB2	0.98
K49HB3	0.99
K49HG2	1.00
K49HD2	1.00
K49HE3	1.00
K49HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS49	HB2	0.99	0.031	0.90	0.00
LYS49	HB3	0.99	0.059	0.01	0.00
LYS49	HG2	1.00	0.007	1.00	1.66
LYS49	HD2	1.00	0.043	0.00	0.00
LYS49	HE2	1.00	0.015	1.00	227.40
LYS49	HA	0.76	0.005	1.00	0.47

3.49.6 Detailed Probabilities of LYS49N:

Overall probability: 0.396

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU48	0.21	1.00
LYS49	0.50	1.00
ASN50	0.70	1.00

Expected NOESY Contacts

Proton	Expected probability
E48HG2	0.98
E48HB2	1.00
E48H	1.00
E48HG3	0.96
E48HA	1.00
K49HA	1.00
K49HB2	1.00
K49HB3	1.00
K49HG2	1.00
K49H	1.00
N50H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU48	HA	1.00	0.009	1.00	-448858.00
GLU48	HB2	1.00	0.134	0.00	0.00
GLU48	HG2	0.98	0.296	0.02	0.00
GLU48	HG3	0.96	0.413	0.04	0.00
GLU48	H	1.00	0.627	0.00	0.00
LYS49	HA	1.00	0.064	0.00	0.00
LYS49	HB2	1.00	0.007	1.00	-198518.00
LYS49	HB3	1.00	0.098	0.00	0.00
LYS49	HG2	1.00	0.003	1.00	-273862.00
LYS49	H	1.00	0.149	0.00	0.00
LYS49	HD2	0.88	0.004	1.00	-74607.00
ASN50	H	1.00	0.033	0.70	0.00

3.49.7 Detailed Probabilities of LYS49HA:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU48	0.67	1.00
LYS49	0.86	1.00
ASN50	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E48HA	1.00
K49HB2	1.00
K49HB3	1.00
K49HG2	1.00
K49HD2	0.98
K49H	1.00
K49HA	1.00
N50H	1.00
N50HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU48	HA	1.00	0.298	0.00	0.00
GLU48	HB2	0.64	0.020	1.00	2.30
GLU48	H	0.88	0.013	1.00	-830971.00
LYS49	HA	1.00	0.008	1.00	21.81
LYS49	HB2	1.00	0.012	1.00	1.59
LYS49	HB3	1.00	0.001	1.00	0.61
LYS49	HG2	1.00	0.003	1.00	0.81
LYS49	HD2	0.98	0.007	1.00	1.05
LYS49	H	1.00	0.064	0.00	0.00
LYS49	HE2	0.77	0.005	1.00	0.47
ASN50	HA	1.00	0.101	0.00	0.00
ASN50	H	1.00	0.593	0.00	0.00

3.49.8 Detailed Probabilities of LYS49HB2:

Overall probability: 0.878

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS49	0.84	1.00
ASN50	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K49HA	1.00
K49HB3	1.00
K49HG2	1.00
K49HD2	1.00
K49HE2	0.98
K49H	1.00
K49HB2	1.00
N50H	1.00

NOESY contacts detailed probability

3.49 LYS(49)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS49	HA	1.00	0.002	1.00	1.31
LYS49	HB2	1.00	0.005	1.00	53.87
LYS49	HB3	1.00	0.019	1.00	4.54
LYS49	HG2	1.00	0.007	1.00	2.94
LYS49	HD2	1.00	0.215	0.00	0.00
LYS49	HE2	0.98	0.031	0.90	0.00
LYS49	H	1.00	0.007	1.00	-198518.00
ASN50	H	1.00	0.020	1.00	-214688.00
ASN50	HA	0.61	0.005	1.00	0.12

3.49.9 Detailed Probabilities of LYS49HB3:

Overall probability: 0.512

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS49	0.52	1.00
ASN50	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K49HA	1.00
K49HB2	1.00
K49HG2	1.00
K49HD2	1.00
K49HE2	0.99
K49H	1.00
K49HB3	1.00
N50H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS49	HA	1.00	0.010	1.00	0.70
LYS49	HB2	1.00	0.010	1.00	5.01
LYS49	HB3	1.00	0.013	1.00	9.08
LYS49	HG2	1.00	0.034	0.60	0.00
LYS49	HD2	1.00	0.071	0.00	0.00
LYS49	HE2	0.99	0.059	0.01	0.00
LYS49	H	1.00	0.098	0.00	0.00
ASN50	H	1.00	0.061	0.00	0.00
ASN50	HB2	0.51	0.015	1.00	0.07

3.49.10 Detailed Probabilities of LYS49HG2:

Overall probability: 0.644

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS49	0.73	0.88
ASN50	0.05	1.00

Expected NOESY Contacts

Proton	Expected probability
K49HA	1.00
K49HB2	1.00
K49HB3	1.00
K49HG3	1.00
K49HD2	1.00
K49HE2	1.00
K49H	1.00
K49HZ2	1.00
N50H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS49	HA	1.00	0.207	0.00	0.00
LYS49	HB2	1.00	0.015	1.00	3.41
LYS49	HB3	1.00	0.009	1.00	1.38
LYS49	HG2	1.00	0.011	1.00	52.13
LYS49	HD2	1.00	0.039	0.10	0.00
LYS49	HE2	1.00	0.007	1.00	1.66
LYS49	H	1.00	0.003	1.00	-273862.00
ASN50	H	0.95	0.236	0.05	0.00

3.49.11 Detailed Probabilities of LYS49HD2:

Overall probability: 0.560

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS49	0.56	0.86

Expected NOESY Contacts

Proton	Expected probability
K49HA	0.98
K49HB2	1.00
K49HB3	1.00
K49HG2	1.00
K49HD3	1.00
K49HE2	1.00
K49HZ2	1.00

NOESY contacts detailed probability

3.49 LYS(49)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS49	HA	0.98	0.112	0.02	0.00
LYS49	HB2	1.00	0.030	1.00	0.00
LYS49	HB3	1.00	0.115	0.00	0.00
LYS49	HG2	1.00	0.029	1.00	6.34
LYS49	HD2	1.00	0.031	0.90	0.00
LYS49	HE2	1.00	0.043	0.00	0.00
LYS49	H	0.87	0.004	1.00	-74607.00

3.49.12 Detailed Probabilities of LYS49HE2:

Overall probability: 0.543

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS49	0.54	0.83

Expected NOESY Contacts

Proton	Expected probability
K49HB2	0.98
K49HB3	0.99
K49HG2	1.00
K49HD2	1.00
K49HE3	1.00
K49HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS49	HB2	0.98	0.086	0.02	0.00
LYS49	HB3	0.99	0.008	1.00	0.12
LYS49	HG2	1.00	0.055	0.00	0.00
LYS49	HD2	1.00	0.033	0.70	0.00
LYS49	HE2	1.00	0.015	1.00	227.40

3.49.13 Detailed Probabilities of LYS49H:

Overall probability: 0.735

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU48	0.56	1.00
LYS49	0.83	1.00
ASN50	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E48HG2	0.98
E48HB2	1.00
E48H	1.00
E48HG3	0.96
E48HA	1.00
K49HA	1.00
K49HB2	1.00
K49HB3	1.00
K49HG2	1.00
K49H	1.00
N50H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU48	HA	1.00	0.005	1.00	0.54
GLU48	HB2	1.00	0.033	0.70	0.00
GLU48	HG2	0.98	0.089	0.02	0.00
GLU48	HG3	0.96	0.039	0.10	0.00
GLU48	H	1.00	0.005	1.00	-121353.00
LYS49	HA	1.00	0.023	1.00	0.57
LYS49	HB2	1.00	0.002	1.00	0.34
LYS49	HB3	1.00	0.000	1.00	0.57
LYS49	HG2	1.00	0.005	1.00	0.22
LYS49	H	1.00	0.149	0.00	0.00
LYS49	HD2	0.88	0.003	1.00	0.26
ASN50	H	1.00	0.006	1.00	-115614.00

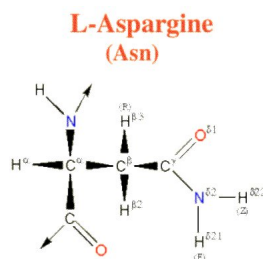
3.50 ASN(50)

Figure 49: Image from the BMRB

Residue probability: 0.717

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	176.454	175.315	1.862	0.000	0.000
CA 3.50.1	53.555	53.674	5.429	0.600	1.000
CB 3.50.2	39.036	38.785	5.449	1.000	1.000
N 3.50.3	117.993	118.907	6.480	0.278	1.000
ND2 3.50.4	113.384	112.932	14.355	1.000	1.000
HA 3.50.5	4.624	4.658	0.371	0.667	1.000
HB2 3.50.6	2.706	2.800	0.341	0.757	1.000
HB3 3.50.7	2.707	2.739	0.364	0.757	1.000
H 3.50.8	8.723	8.328	0.633	0.644	1.000
HD21 3.50.9	7.633	7.343	1.188	0.671	1.000
HD22 3.50.10	6.878	7.145	1.184	0.800	1.000

3.50.1 Detailed Probabilities of ASN50CA:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS49	0.50	1.00
ASN50	0.67	1.00
PHE51	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K49HA	1.00
N50HB2	1.00
N50HB3	1.00
N50H	1.00
N50HD21	1.00
N50HD22	1.00
N50HA	1.00
F51HA	1.00
F51H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS49	HA	1.00	0.101	0.00	0.00
LYS49	HB2	0.61	0.005	1.00	0.12
ASN50	HA	1.00	0.006	1.00	8.70
ASN50	HB2	1.00	0.002	1.00	1.71
ASN50	HB3	1.00	0.003	1.00	1.71
ASN50	H	1.00	0.019	1.00	0.35
ASN50	HD21	1.00	0.180	0.00	0.00
ASN50	HD22	1.00	0.149	0.00	0.00
PHE51	HA	1.00	0.057	0.00	0.00
PHE51	H	1.00	0.010	1.00	0.76

3.50.2 Detailed Probabilities of ASN50CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN50	1.00	1.00
PHE51	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N50HA	1.00
N50HB3	1.00
N50H	1.00
N50HD21	1.00
N50HD22	1.00
N50HB2	1.00
F51H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN50	HA	1.00	0.008	1.00	1.18
ASN50	HB2	1.00	0.000	1.00	15.99
ASN50	HB3	1.00	0.001	1.00	15.99
ASN50	H	1.00	0.022	1.00	0.38
ASN50	HD21	1.00	0.004	1.00	0.54
ASN50	HD22	1.00	0.003	1.00	0.32
PHE51	H	1.00	0.011	1.00	0.47

3.50.3 Detailed Probabilities of ASN50N:

Overall probability: 0.278

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS49	0.41	1.00
ASN50	0.00	1.00
PHE51	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K49HB3	1.00
K49HG2	0.97
K49HA	1.00
K49HB2	1.00
K49H	1.00
N50HA	1.00
N50HB2	1.00
N50HB3	1.00
N50HD21	0.98
N50H	1.00
F51H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS49	HA	1.00	0.593	0.00	0.00
LYS49	HB2	1.00	0.020	1.00	-214688.00
LYS49	HB3	1.00	0.061	0.00	0.00
LYS49	HG2	0.97	0.236	0.03	0.00
LYS49	H	1.00	0.006	1.00	-115614.00
ASN50	HA	1.00	0.287	0.00	0.00
ASN50	HB2	1.00	0.787	0.00	0.00
ASN50	HB3	1.00	0.788	0.00	0.00
ASN50	H	1.00	0.110	0.00	0.00
ASN50	HD21	0.98	0.041	0.02	0.00
PHE51	H	1.00	0.013	1.00	-139450.00

3.50.4 Detailed Probabilities of ASN50ND2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN50	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N50HA	1.00
N50HB2	1.00
N50HB3	1.00
N50HD21	1.00
N50HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN50	HA	1.00	0.008	1.00	-98622.00
ASN50	HB2	1.00	0.000	1.00	-565594.00
ASN50	HB3	1.00	0.001	1.00	-565594.00
ASN50	HD21	1.00	0.002	1.00	-6205190.00
ASN50	HD22	1.00	0.007	1.00	-10491945.00

3.50.5 Detailed Probabilities of ASN50HA:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS49	1.00	1.00
ASN50	0.67	1.00
PHE51	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K49HA	1.00
N50HB2	1.00
N50HB3	1.00
N50H	1.00
N50HD21	1.00
N50HD22	1.00
N50HA	1.00
F51HA	1.00
F51H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS49	HA	1.00	0.013	1.00	0.12
ASN50	HA	1.00	0.006	1.00	8.70
ASN50	HB2	1.00	0.008	1.00	1.18
ASN50	HB3	1.00	0.008	1.00	1.18
ASN50	H	1.00	0.287	0.00	0.00
ASN50	HD21	1.00	0.052	0.00	0.00
ASN50	HD22	1.00	0.008	1.00	-98622.00
PHE51	HA	1.00	0.243	0.00	0.00
PHE51	H	1.00	0.007	1.00	-839044.00

3.50.6 Detailed Probabilities of ASN50HB2:

Overall probability: 0.757

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN50	0.83	1.00
PHE51	0.30	1.00

Expected NOESY Contacts

Proton	Expected probability
N50HA	1.00
N50HB3	1.00
N50H	1.00
N50HD21	1.00
N50HD22	1.00
N50HB2	1.00
F51H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN50	HA	1.00	0.003	1.00	1.71
ASN50	HB2	1.00	0.001	1.00	15.99
ASN50	HB3	1.00	0.001	1.00	15.99
ASN50	H	1.00	0.787	0.00	0.00
ASN50	HD21	1.00	0.000	1.00	-712768.00
ASN50	HD22	1.00	0.001	1.00	-565594.00
PHE51	H	1.00	0.037	0.30	0.00

3.50.7 Detailed Probabilities of ASN50HB3:

Overall probability: 0.757

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN50	0.83	1.00
PHE51	0.30	1.00

Expected NOESY Contacts

Proton	Expected probability
N50HA	1.00
N50HB2	1.00
N50H	1.00
N50HD21	1.00
N50HD22	1.00
N50HB3	1.00
F51H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN50	HA	1.00	0.003	1.00	1.71
ASN50	HB2	1.00	0.001	1.00	15.99
ASN50	HB3	1.00	0.001	1.00	15.99
ASN50	H	1.00	0.787	0.00	0.00
ASN50	HD21	1.00	0.000	1.00	-712768.00
ASN50	HD22	1.00	0.001	1.00	-565594.00
PHE51	H	1.00	0.037	0.30	0.00

3.50.8 Detailed Probabilities of ASN50H:

Overall probability: 0.644

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS49	0.62	1.00
ASN50	0.60	1.00
PHE51	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K49HB3	1.00
K49HG2	0.97
K49HA	1.00
K49HB2	1.00
K49H	1.00
N50HA	1.00
N50HB2	1.00
N50HB3	1.00
N50HD21	0.98
N50H	1.00
F51H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS49	HA	1.00	0.093	0.00	0.00
LYS49	HB2	1.00	1.032	0.00	0.00
LYS49	HB3	1.00	0.003	1.00	0.07
LYS49	HG2	0.97	0.003	1.00	0.07
LYS49	H	1.00	0.033	0.70	0.00
LYS49	HD2	0.56	0.009	1.00	0.29
ASN50	HA	1.00	0.019	1.00	0.35
ASN50	HB2	1.00	0.022	1.00	0.38
ASN50	HB3	1.00	0.022	1.00	0.38
ASN50	H	1.00	0.110	0.00	0.00
ASN50	HD21	0.98	1.087	0.02	0.00
PHE51	H	1.00	0.017	1.00	-96551.00

3.50.9 Detailed Probabilities of ASN50HD21:

Overall probability: 0.671

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN50	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
N50HA	1.00
N50HB2	1.00
N50HB3	1.00
N50H	0.98
N50HD22	1.00
N50HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN50	HA	1.00	0.180	0.00	0.00
ASN50	HB2	1.00	0.004	1.00	0.54
ASN50	HB3	1.00	0.004	1.00	0.54
ASN50	H	0.98	0.041	0.02	0.00
ASN50	HD21	1.00	0.003	1.00	-6497528.00
ASN50	HD22	1.00	0.002	1.00	-6205190.00

3.50.10 Detailed Probabilities of ASN50HD22:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN50	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
N50HA	1.00
N50HB2	1.00
N50HB3	1.00
N50HD21	1.00
N50HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN50	HA	1.00	0.149	0.00	0.00
ASN50	HB2	1.00	0.003	1.00	0.32
ASN50	HB3	1.00	0.003	1.00	0.32
ASN50	HD21	1.00	0.005	1.00	-5903898.00
ASN50	HD22	1.00	0.007	1.00	-10491945.00

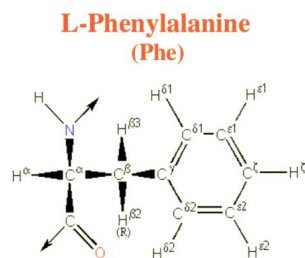


Figure 50: Image from the BMRB

Residue probability: 0.534
Residue probability confidence: 0.833

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	NA	—	—	0.000	0.000
CA 3.51.1	57.935	58.245	3.808	0.000	0.889
CB 3.51.2	38.975	40.078	3.616	0.717	0.857
CD1 3.51.3	131.731	131.234	9.579	0.667	0.750
CD2 3.51.4	131.836	131.352	9.581	0.336	0.750
CE1	NA	—	—	0.000	0.000
CE2	NA	—	—	0.000	0.000
CZ	NA	—	—	0.000	0.000
N 3.51.5	120.700	120.315	4.931	0.840	0.909
HA 3.51.6	4.758	4.625	1.237	0.463	0.889
HB2 3.51.7	3.027	2.980	0.399	0.333	0.857
HB3 3.51.8	2.967	2.916	0.434	0.483	0.857
HD1 3.51.9	7.124	7.037	0.347	0.667	0.750
HD2 3.51.10	7.124	7.022	0.417	0.667	0.750
HE	NA	—	—	0.000	0.000
HZ	NA	—	—	0.000	0.000
H 3.51.11	8.341	8.375	0.710	0.701	0.909

3.51.1 Detailed Probabilities of PHE51CA:

Overall probability: 0.000
Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN50	0.00	1.00
PHE51	0.00	1.00
GLU52	0.00	0.50

Expected NOESY Contacts

Proton	Expected probability
N50HA	1.00
F51HB2	1.00
F51HB3	1.00
F51HD1	1.00
F51HD2	1.00
F51H	1.00
F51HA	1.00
E52H	1.00
E52HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN50	HA	1.00	0.243	0.00	0.00
PHE51	HA	1.00	0.109	0.00	0.00
PHE51	HB2	1.00	0.140	0.00	0.00
PHE51	HB3	1.00	0.080	0.00	0.00
PHE51	HD1	1.00	0.047	0.00	0.00
PHE51	HD2	1.00	0.047	0.00	0.00
PHE51	H	1.00	0.097	0.00	0.00
GLU52	HA	1.00	0.609	0.00	0.00

3.51.2 Detailed Probabilities of PHE51CB:

Overall probability: 0.717

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE51	0.72	1.00
GLU52	0.00	0.00

Expected NOESY Contacts

Proton	Expected probability
F51HA	1.00
F51HB3	1.00
F51HD1	1.00
F51HD2	1.00
F51H	1.00
F51HB2	1.00
E52H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE51	HA	1.00	0.037	0.30	0.00
PHE51	HB2	1.00	0.007	1.00	4.05
PHE51	HB3	1.00	0.053	0.00	0.00
PHE51	HD1	1.00	0.009	1.00	0.43
PHE51	HD2	1.00	0.009	1.00	0.43
PHE51	H	1.00	0.018	1.00	0.38

3.51.3 Detailed Probabilities of PHE51CD1:

Overall probability: 0.667

Overall confidence: 0.750

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE51	0.67	0.75

Expected NOESY Contacts

Proton	Expected probability
F51HA	1.00
F51HB2	1.00
F51HB3	1.00
F51HD2	1.00
F51HE1	1.00
F51HZ	1.00
F51H	1.00
F51HD1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE51	HA	1.00	0.013	1.00	0.44
PHE51	HB2	1.00	0.058	0.00	0.00
PHE51	HB3	1.00	0.002	1.00	0.53
PHE51	HD1	1.00	0.019	1.00	24.03
PHE51	HD2	1.00	0.019	1.00	24.03
PHE51	H	1.00	1.548	0.00	0.00

3.51.4 Detailed Probabilities of PHE51CD2:

Overall probability: 0.336

Overall confidence: 0.750

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE51	0.34	0.75

Expected NOESY Contacts

Proton	Expected probability
F51HA	1.00
F51HB2	1.00
F51HB3	1.00
F51HD1	1.00
F51HE1	1.00
F51HZ	1.00
F51H	0.99
F51HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE51	HA	1.00	0.013	1.00	0.44
PHE51	HB2	1.00	0.058	0.00	0.00
PHE51	HB3	1.00	0.002	1.00	0.53
PHE51	HD1	1.00	0.331	0.00	0.00
PHE51	HD2	1.00	0.331	0.00	0.00
PHE51	H	0.99	1.548	0.01	0.00

3.51.5 Detailed Probabilities of PHE51N:

Overall probability: 0.840

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN50	0.62	1.00
PHE51	0.98	1.00
GLU52	NaN	0.00

Expected NOESY Contacts

Proton	Expected probability
N50HB3	1.00
N50HB2	1.00
N50H	1.00
N50HA	1.00
F51HA	1.00
F51HB2	1.00
F51HB3	1.00
F51HD1	1.00
F51HD2	0.99
F51H	1.00
E52H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN50	HA	1.00	0.007	1.00	-839044.00
ASN50	HB2	1.00	0.038	0.20	0.00
ASN50	HB3	1.00	0.037	0.30	0.00
ASN50	H	1.00	0.017	1.00	-96551.00
PHE51	HA	1.00	0.030	1.00	0.00
PHE51	HB2	1.00	0.001	1.00	-973176.00
PHE51	HB3	1.00	0.031	0.90	0.00
PHE51	HD1	1.00	0.003	1.00	-161533.00
PHE51	HD2	0.99	0.003	1.00	-161533.00
PHE51	H	1.00	0.030	1.00	0.00

3.51.6 Detailed Probabilities of PHE51HA:

Overall probability: 0.463

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN50	0.00	1.00
PHE51	0.55	1.00
GLU52	0.40	0.50

Expected NOESY Contacts

Proton	Expected probability
N50HA	1.00
F51HB2	1.00
F51HB3	1.00
F51HD1	1.00
F51HD2	1.00
F51H	1.00
F51HA	1.00
E52H	1.00
E52HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN50	HA	1.00	0.057	0.00	0.00
PHE51	HA	1.00	0.109	0.00	0.00
PHE51	HB2	1.00	0.037	0.30	0.00
PHE51	HB3	1.00	0.098	0.00	0.00
PHE51	HD1	1.00	0.013	1.00	0.44
PHE51	HD2	1.00	0.013	1.00	0.44
PHE51	H	1.00	0.030	1.00	0.00
GLU52	HA	1.00	0.036	0.40	0.00

3.51.7 Detailed Probabilities of PHE51HB2:

Overall probability: 0.333

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE51	0.33	1.00
GLU52	0.00	0.00

Expected NOESY Contacts

Proton	Expected probability
F51HA	1.00
F51HB3	1.00
F51HD1	1.00
F51HD2	1.00
F51H	1.00
F51HB2	1.00
E52H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE51	HA	1.00	0.140	0.00	0.00
PHE51	HB2	1.00	0.007	1.00	4.05
PHE51	HB3	1.00	1.127	0.00	0.00
PHE51	HD1	1.00	0.058	0.00	0.00
PHE51	HD2	1.00	0.058	0.00	0.00
PHE51	H	1.00	0.001	1.00	-973176.00

3.51.8 Detailed Probabilities of PHE51HB3:

Overall probability: 0.483

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE51	0.48	1.00
GLU52	0.00	0.00

Expected NOESY Contacts

Proton	Expected probability
F51HA	1.00
F51HB2	1.00
F51HD1	1.00
F51HD2	1.00
F51H	1.00
F51HB3	1.00
E52H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE51	HA	1.00	0.080	0.00	0.00
PHE51	HB2	1.00	0.053	0.00	0.00
PHE51	HB3	1.00	1.067	0.00	0.00
PHE51	HD1	1.00	0.002	1.00	0.53
PHE51	HD2	1.00	0.002	1.00	0.53
PHE51	H	1.00	0.031	0.90	0.00

3.51.9 Detailed Probabilities of PHE51HD1:

Overall probability: 0.667

Overall confidence: 0.750

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE51	0.67	0.75

Expected NOESY Contacts

Proton	Expected probability
F51HA	1.00
F51HB2	1.00
F51HB3	1.00
F51HD2	1.00
F51HE1	1.00
F51HZ	1.00
F51H	1.00
F51HD1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE51	HA	1.00	0.047	0.00	0.00
PHE51	HB2	1.00	0.009	1.00	0.43
PHE51	HB3	1.00	0.005	1.00	0.36
PHE51	HD1	1.00	0.019	1.00	24.03
PHE51	HD2	1.00	0.331	0.00	0.00
PHE51	H	1.00	0.003	1.00	-161533.00

3.51.10 Detailed Probabilities of PHE51HD2:

Overall probability: 0.667

Overall confidence: 0.750

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE51	0.67	0.75

Expected NOESY Contacts

Proton	Expected probability
F51HA	1.00
F51HB2	1.00
F51HB3	1.00
F51HD1	1.00
F51HE1	1.00
F51HZ	1.00
F51H	0.99
F51HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE51	HA	1.00	0.047	0.00	0.00
PHE51	HB2	1.00	0.009	1.00	0.43
PHE51	HB3	1.00	0.005	1.00	0.36
PHE51	HD1	1.00	0.019	1.00	24.03
PHE51	HD2	1.00	0.331	0.00	0.00
PHE51	H	0.99	0.003	1.00	-161533.00

3.51.11 Detailed Probabilities of PHE51H:

Overall probability: 0.701

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN50	1.00	1.00
PHE51	0.50	1.00
GLU52	0.00	0.00

Expected NOESY Contacts

Proton	Expected probability
N50HB3	1.00
N50HB2	1.00
N50H	1.00
N50HA	1.00
F51HA	1.00
F51HB2	1.00
F51HB3	1.00
F51HD1	1.00
F51HD2	0.99
F51H	1.00
E52H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN50	HA	1.00	0.010	1.00	0.76
ASN50	HB2	1.00	0.011	1.00	0.47
ASN50	HB3	1.00	0.011	1.00	0.47
ASN50	H	1.00	0.013	1.00	-139450.00
PHE51	HA	1.00	0.097	0.00	0.00
PHE51	HB2	1.00	0.018	1.00	0.38
PHE51	HB3	1.00	0.026	1.00	0.14
PHE51	HD1	1.00	1.548	0.00	0.00
PHE51	HD2	0.99	1.548	0.01	0.00
PHE51	H	1.00	0.030	1.00	0.00

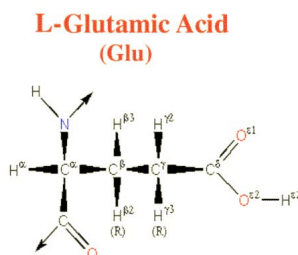


Figure 51: Image from the BMRB

Residue probability: 0.470
Residue probability confidence: 0.785

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	173.600	176.942	2.547	0.000	0.000
CA 3.52.1	56.254	57.442	3.837	0.263	0.889
CB 3.52.2	33.459	30.185	4.018	0.817	0.750
CG 3.52.3	36.666	36.085	1.533	0.500	0.750
N	NA	—	—	0.000	0.000
HA 3.52.4	4.258	4.245	0.429	0.667	0.889
HB2 3.52.5	1.656	2.021	0.233	0.714	0.750
HB3 3.52.6	1.952	1.994	0.244	0.167	0.750
HG2 3.52.7	2.100	2.258	0.226	0.317	0.750
HG3 3.52.8	2.044	2.233	0.232	0.317	0.750
H	NA	—	—	0.000	0.000
HE2	NA	—	—	0.000	0.000

3.52.1 Detailed Probabilities of GLU52CA:

Overall probability: 0.263
Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE51	0.40	1.00
GLU52	0.00	0.83
LYS53	0.85	1.00

Expected NOESY Contacts

Proton	Expected probability
F51HA	1.00
E52HB2	1.00
E52HB3	1.00
E52HG2	1.00
E52HG3	1.00
E52H	1.00
E52HA	1.00
K53HA	1.00
K53H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE51	HA	1.00	0.036	0.40	0.00
GLU52	HA	1.00	0.464	0.00	0.00
GLU52	HB2	1.00	0.589	0.00	0.00
GLU52	HB3	1.00	0.729	0.00	0.00
GLU52	HG2	1.00	0.581	0.00	0.00
GLU52	HG3	1.00	0.637	0.00	0.00
LYS53	HA	1.00	0.033	0.70	0.00
LYS53	H	1.00	0.009	1.00	0.75

3.52.2 Detailed Probabilities of GLU52CB:

Overall probability: 0.817

Overall confidence: 0.750

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU52	0.78	0.71
LYS53	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E52HA	1.00
E52HB3	1.00
E52HG2	1.00
E52HG3	1.00
E52H	1.00
E52HE2	1.00
E52HB2	1.00
K53H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU52	HA	1.00	0.007	1.00	0.17
GLU52	HB2	1.00	0.020	1.00	1.51
GLU52	HB3	1.00	0.123	0.00	0.00
GLU52	HG2	1.00	0.025	1.00	0.34
GLU52	HG3	1.00	0.031	0.90	0.00
LYS53	H	1.00	0.005	1.00	0.09

3.52.3 Detailed Probabilities of GLU52CG:

Overall probability: 0.500

Overall confidence: 0.750

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU52	0.40	0.71
LYS53	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E52HA	1.00
E52HB2	1.00
E52HB3	1.00
E52HG2	1.00
E52H	1.00
E52HE2	1.00
E52HG3	1.00
K53H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU52	HA	1.00	0.003	1.00	0.30
GLU52	HB2	1.00	0.006	1.00	0.39
GLU52	HB3	1.00	0.187	0.00	0.00
GLU52	HG2	1.00	0.280	0.00	0.00
GLU52	HG3	1.00	0.279	0.00	0.00
LYS53	H	0.96	0.001	1.00	0.07

3.52.4 Detailed Probabilities of GLU52HA:

Overall probability: 0.667

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE51	0.50	1.00
GLU52	0.60	0.83
LYS53	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F51HA	1.00
E52HB2	1.00
E52HB3	1.00
E52HG2	1.00
E52HG3	1.00
E52H	1.00
E52HA	1.00
K53HA	1.00
K53H	1.00

NOESY contacts detailed probability

3.52 GLU(52)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE51	HA	1.00	0.609	0.00	0.00
PHE51	H	0.90	0.025	1.00	-103502.00
GLU52	HA	1.00	0.464	0.00	0.00
GLU52	HB2	1.00	0.007	1.00	0.17
GLU52	HB3	1.00	0.000	1.00	0.32
GLU52	HG2	1.00	2.599	0.00	0.00
GLU52	HG3	1.00	0.003	1.00	0.30
LYS53	HA	1.00	0.023	1.00	0.25
LYS53	H	1.00	0.004	1.00	-972184.00

3.52.5 Detailed Probabilities of GLU52HB2:

Overall probability: 0.714

Overall confidence: 0.750

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU52	0.60	0.71
LYS53	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E52HA	1.00
E52HB3	1.00
E52HG2	1.00
E52HG3	1.00
E52H	1.00
E52HE2	1.00
E52HB2	1.00
K53H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU52	HA	1.00	0.589	0.00	0.00
GLU52	HB2	1.00	0.020	1.00	1.51
GLU52	HB3	1.00	0.538	0.00	0.00
GLU52	HG2	1.00	0.003	1.00	0.32
GLU52	HG3	1.00	0.006	1.00	0.39
LYS53	H	1.00	0.009	1.00	-230015.00
LYS53	HA	0.64	0.010	1.00	0.37

3.52.6 Detailed Probabilities of GLU52HB3:

Overall probability: 0.167

Overall confidence: 0.750

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU52	0.00	0.71
LYS53	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E52HA	1.00
E52HB2	1.00
E52HG2	1.00
E52HG3	1.00
E52H	1.00
E52HE2	1.00
E52HB3	1.00
K53H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU52	HA	1.00	0.729	0.00	0.00
GLU52	HB2	1.00	0.123	0.00	0.00
GLU52	HB3	1.00	0.688	0.00	0.00
GLU52	HG2	1.00	0.293	0.00	0.00
GLU52	HG3	1.00	0.187	0.00	0.00
LYS53	H	1.00	0.005	1.00	-348647.00

3.52.7 Detailed Probabilities of GLU52HG2:

Overall probability: 0.317

Overall confidence: 0.750

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU52	0.20	0.71
LYS53	0.90	1.00

Expected NOESY Contacts

Proton	Expected probability
E52HA	1.00
E52HB2	1.00
E52HB3	1.00
E52HG3	1.00
E52H	1.00
E52HE2	1.00
E52HG2	1.00
K53H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU52	HA	1.00	0.581	0.00	0.00
GLU52	HB2	1.00	0.025	1.00	0.34
GLU52	HB3	1.00	0.540	0.00	0.00
GLU52	HG2	1.00	0.441	0.00	0.00
GLU52	HG3	1.00	0.280	0.00	0.00
LYS53	H	0.98	0.031	0.90	0.00

3.52.8 Detailed Probabilities of GLU52HG3:

Overall probability: 0.317

Overall confidence: 0.750

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU52	0.18	0.71
LYS53	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E52HA	1.00
E52HB2	1.00
E52HB3	1.00
E52HG2	1.00
E52H	1.00
E52HE2	1.00
E52HG3	1.00
K53H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU52	HA	1.00	0.637	0.00	0.00
GLU52	HB2	1.00	0.031	0.90	0.00
GLU52	HB3	1.00	0.596	0.00	0.00
GLU52	HG2	1.00	0.385	0.00	0.00
GLU52	HG3	1.00	0.279	0.00	0.00
LYS53	H	0.96	0.017	1.00	-179410.00

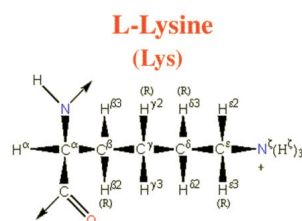


Figure 52: Image from the BMRB

Residue probability: 0.747
Residue probability confidence: 0.935

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.430	176.660	3.133	0.000	0.000
CA 3.53.1	55.356	57.014	3.028	0.694	1.000
CB 3.53.2	31.445	32.981	3.186	0.819	1.000
CG 3.53.3	24.593	24.941	1.956	0.885	0.917
CD 3.53.4	28.780	29.020	2.193	0.802	0.900
CE 3.53.5	41.700	41.893	1.492	0.875	0.889
N 3.53.6	119.964	120.954	4.210	0.993	0.923
NZ	NA	—	—	0.000	0.000
HA 3.53.7	4.689	4.262	0.489	0.718	1.000
HB2 3.53.8	0.111	1.774	0.365	0.820	1.000
HB3 3.53.9	1.130	1.742	0.385	0.428	1.000
HG2 3.53.10	1.087	1.358	0.344	0.636	0.917
HG3 3.53.11	0.935	1.343	0.357	0.818	0.917
HD2 3.53.12	1.480	1.614	0.957	0.700	0.900
HD3 3.53.13	1.268	1.595	0.387	0.902	0.900
HE2 3.53.14	2.628	2.907	0.230	0.627	0.889
HE3 3.53.15	2.717	2.901	0.241	0.378	0.889
H 3.53.16	7.962	8.185	0.605	0.859	0.923
HZ	NA	—	—	0.000	0.000

3.53.1 Detailed Probabilities of LYS53CA:

Overall probability: 0.694
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU52	1.00	1.00
LYS53	0.50	1.00
ILE54	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E52HA	1.00
K53HB2	1.00
K53HB3	1.00
K53HG2	1.00
K53HG3	1.00
K53HD2	0.98
K53HD3	0.98
K53H	1.00
K53HA	1.00
I54HA	1.00
I54H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU52	HA	1.00	0.023	1.00	0.25
GLU52	HB2	0.64	0.010	1.00	0.37
LYS53	HA	1.00	0.146	0.00	0.00
LYS53	HB2	1.00	0.045	0.00	0.00
LYS53	HB3	1.00	0.040	0.00	0.00
LYS53	HG2	1.00	0.001	1.00	0.45
LYS53	HG3	1.00	0.006	1.00	0.24
LYS53	HD2	0.98	0.013	1.00	0.49
LYS53	HD3	0.98	0.076	0.02	0.00
LYS53	H	1.00	0.017	1.00	0.36
ILE54	HA	1.00	0.011	1.00	0.42
ILE54	H	1.00	0.017	1.00	0.35
ILE54	HG13	0.65	0.018	1.00	0.24

3.53.2 Detailed Probabilities of LYS53CB:

Overall probability: 0.819

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS53	0.80	1.00
ILE54	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K53HA	1.00
K53HB2	1.00
K53HG2	1.00
K53HG3	1.00
K53HD2	1.00
K53HD3	1.00
K53HE2	0.99
K53HE3	0.99
K53H	1.00
K53HB3	1.00
I54H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS53	HA	1.00	0.007	1.00	0.12
LYS53	HB2	1.00	0.009	1.00	0.49
LYS53	HB3	1.00	0.002	1.00	0.80
LYS53	HG2	1.00	0.041	0.00	0.00
LYS53	HG3	1.00	0.005	1.00	0.26
LYS53	HD2	1.00	0.005	1.00	0.13
LYS53	HD3	1.00	0.001	1.00	0.16
LYS53	HE2	0.99	0.010	1.00	0.08
LYS53	HE3	0.99	0.079	0.01	0.00
LYS53	H	1.00	0.011	1.00	0.12
ILE54	H	1.00	0.021	1.00	0.06

3.53.3 Detailed Probabilities of LYS53CG:

Overall probability: 0.885

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS53	0.97	0.91
ILE54	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
K53HA	1.00
K53HB2	1.00
K53HB3	1.00
K53HG3	1.00
K53HD2	1.00
K53HD3	1.00
K53HE2	1.00
K53HE3	1.00
K53H	1.00
K53HZ2	1.00
K53HG2	1.00
I54H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS53	HA	1.00	0.010	1.00	0.08
LYS53	HB2	1.00	0.006	1.00	0.14
LYS53	HB3	1.00	0.033	0.70	0.00
LYS53	HG2	1.00	0.010	1.00	1.55
LYS53	HG3	1.00	0.001	1.00	1.05
LYS53	HD2	1.00	0.004	1.00	0.28
LYS53	HD3	1.00	0.008	1.00	0.51
LYS53	HE2	1.00	0.006	1.00	0.10
LYS53	HE3	1.00	0.001	1.00	0.07
LYS53	H	1.00	0.005	1.00	0.15
ILE54	H	0.97	0.837	0.03	0.00

3.53.4 Detailed Probabilities of LYS53CD:

Overall probability: 0.802

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS53	0.80	0.90

Expected NOESY Contacts

Proton	Expected probability
K53HA	0.98
K53HB2	1.00
K53HB3	1.00
K53HG2	1.00
K53HG3	1.00
K53HD2	1.00
K53HE2	1.00
K53HE3	1.00
K53HZ2	1.00
K53HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS53	HA	0.98	0.043	0.02	0.00
LYS53	HB2	1.00	0.006	1.00	0.14
LYS53	HB3	1.00	0.044	0.00	0.00
LYS53	HG2	1.00	0.001	1.00	1.16
LYS53	HG3	1.00	0.023	1.00	1.39
LYS53	HD2	1.00	0.002	1.00	2.28
LYS53	HD3	1.00	0.002	1.00	6.06
LYS53	HE2	1.00	0.016	1.00	0.25
LYS53	HE3	1.00	0.009	1.00	0.43
LYS53	H	0.87	0.011	1.00	0.06

3.53.5 Detailed Probabilities of LYS53CE:

Overall probability: 0.875

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS53	0.88	0.89

Expected NOESY Contacts

Proton	Expected probability
K53HB2	0.99
K53HB3	0.99
K53HG2	1.00
K53HG3	1.00
K53HD2	1.00
K53HD3	1.00
K53HE2	1.00
K53HZ2	1.00
K53HE3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS53	HB2	0.99	0.010	1.00	0.06
LYS53	HB3	0.99	0.030	1.00	1.02
LYS53	HG2	1.00	0.013	1.00	1.02
LYS53	HG3	1.00	0.030	1.00	0.17
LYS53	HD2	1.00	0.007	1.00	0.45
LYS53	HD3	1.00	0.002	1.00	0.50
LYS53	HE2	1.00	0.078	0.00	0.00
LYS53	HE3	1.00	0.011	1.00	27.21

3.53.6 Detailed Probabilities of LYS53N:

Overall probability: 0.993

Overall confidence: 0.923

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU52	0.98	0.83
LYS53	1.00	1.00
ILE54	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E52HG2	0.98
E52HB2	1.00
E52H	1.00
E52HG3	0.96
E52HB3	1.00
E52HA	1.00
K53HA	1.00
K53HB2	1.00
K53HB3	1.00
K53HG2	1.00
K53HG3	1.00
K53H	1.00
I54H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU52	HA	1.00	0.004	1.00	-972184.00
GLU52	HB2	1.00	0.009	1.00	-230015.00
GLU52	HB3	1.00	0.005	1.00	-348647.00
GLU52	HG2	0.98	0.031	0.90	0.00
GLU52	HG3	0.96	0.017	1.00	-179410.00
LYS53	HA	1.00	0.008	1.00	-186222.00
LYS53	HB2	1.00	0.013	1.00	-112245.00
LYS53	HB3	1.00	0.017	1.00	-488946.00
LYS53	HG2	1.00	0.026	1.00	-488946.00
LYS53	HG3	1.00	0.006	1.00	-243009.00
LYS53	H	1.00	0.008	1.00	-5054351.00
LYS53	HD2	0.88	0.015	1.00	-72527.00
LYS53	HD3	0.87	0.004	1.00	-119128.00
ILE54	H	1.00	0.003	1.00	-137837.00
ILE54	HG13	0.59	0.030	1.00	-243009.00

3.53.7 Detailed Probabilities of LYS53HA:

Overall probability: 0.718

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU52	0.70	1.00
LYS53	0.77	1.00
ILE54	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E52HA	1.00
K53HB2	1.00
K53HB3	1.00
K53HG2	1.00
K53HG3	1.00
K53HD2	0.98
K53HD3	0.98
K53H	1.00
K53HA	1.00
I54HA	1.00
I54H	1.00

NOESY contacts detailed probability

3.53 LYS(53)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU52	HA	1.00	0.033	0.70	0.00
LYS53	HA	1.00	0.146	0.00	0.00
LYS53	HB2	1.00	0.002	1.00	0.08
LYS53	HB3	1.00	0.007	1.00	0.12
LYS53	HG2	1.00	0.010	1.00	0.08
LYS53	HG3	1.00	0.026	1.00	0.07
LYS53	HD2	0.98	0.031	0.90	0.00
LYS53	HD3	0.98	0.043	0.02	0.00
LYS53	H	1.00	0.008	1.00	-186222.00
LYS53	HE2	0.77	0.005	1.00	0.47
ILE54	HA	1.00	0.059	0.00	0.00
ILE54	H	1.00	0.006	1.00	-912658.00

3.53.8 Detailed Probabilities of LYS53HB2:

Overall probability: 0.820

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS53	0.80	1.00
ILE54	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K53HA	1.00
K53HB3	1.00
K53HG2	1.00
K53HG3	1.00
K53HD2	1.00
K53HD3	1.00
K53HE2	0.98
K53HE3	0.99
K53H	1.00
K53HB2	1.00
I54H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS53	HA	1.00	0.045	0.00	0.00
LYS53	HB2	1.00	0.002	1.00	0.26
LYS53	HB3	1.00	0.009	1.00	0.49
LYS53	HG2	1.00	0.006	1.00	0.14
LYS53	HG3	1.00	0.013	1.00	0.06
LYS53	HD2	1.00	0.007	1.00	0.12
LYS53	HD3	1.00	0.006	1.00	0.14
LYS53	HE2	0.98	0.772	0.02	0.00
LYS53	HE3	0.99	0.010	1.00	0.06
LYS53	H	1.00	0.013	1.00	-112245.00
ILE54	H	1.00	0.007	1.00	-93311.00

3.53.9 Detailed Probabilities of LYS53HB3:

Overall probability: 0.428

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS53	0.47	1.00
ILE54	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K53HA	1.00
K53HB2	1.00
K53HG2	1.00
K53HG3	1.00
K53HD2	1.00
K53HD3	1.00
K53HE2	0.99
K53HE3	0.99
K53H	1.00
K53HB3	1.00
I54H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS53	HA	1.00	0.040	0.00	0.00
LYS53	HB2	1.00	0.002	1.00	0.39
LYS53	HB3	1.00	0.002	1.00	0.80
LYS53	HG2	1.00	0.033	0.70	0.00
LYS53	HG3	1.00	0.041	0.00	0.00
LYS53	HD2	1.00	0.139	0.00	0.00
LYS53	HD3	1.00	0.044	0.00	0.00
LYS53	HE2	0.99	0.137	0.01	0.00
LYS53	HE3	0.99	0.030	1.00	1.02
LYS53	H	1.00	0.017	1.00	-488946.00
ILE54	H	1.00	0.044	0.00	0.00

3.53.10 Detailed Probabilities of LYS53HG2:

Overall probability: 0.636

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS53	0.60	0.91
ILE54	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K53HA	1.00
K53HB2	1.00
K53HB3	1.00
K53HG3	1.00
K53HD2	1.00
K53HD3	1.00
K53HE2	1.00
K53HE3	1.00
K53H	1.00
K53HZ2	1.00
K53HG2	1.00
I54H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS53	HA	1.00	0.001	1.00	0.45
LYS53	HB2	1.00	0.045	0.00	0.00
LYS53	HB3	1.00	0.041	0.00	0.00
LYS53	HG2	1.00	0.010	1.00	1.55
LYS53	HG3	1.00	0.002	1.00	1.35
LYS53	HD2	1.00	0.146	0.00	0.00
LYS53	HD3	1.00	0.001	1.00	1.16
LYS53	HE2	1.00	0.180	0.00	0.00
LYS53	HE3	1.00	0.013	1.00	1.02
LYS53	H	1.00	0.026	1.00	-488946.00
ILE54	H	0.97	0.001	1.00	-170001.00

3.53.11 Detailed Probabilities of LYS53HG3:

Overall probability: 0.818

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS53	0.80	0.91
ILE54	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K53HA	1.00
K53HB2	1.00
K53HB3	1.00
K53HG2	1.00
K53HD2	1.00
K53HD3	1.00
K53HE2	1.00
K53HE3	1.00
K53H	1.00
K53HZ2	1.00
K53HG3	1.00
I54H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS53	HA	1.00	0.006	1.00	0.24
LYS53	HB2	1.00	0.008	1.00	0.14
LYS53	HB3	1.00	0.005	1.00	0.26
LYS53	HG2	1.00	0.001	1.00	1.05
LYS53	HG3	1.00	0.154	0.00	0.00
LYS53	HD2	1.00	0.006	1.00	0.46
LYS53	HD3	1.00	0.023	1.00	1.39
LYS53	HE2	1.00	0.332	0.00	0.00
LYS53	HE3	1.00	0.030	1.00	0.17
LYS53	H	1.00	0.006	1.00	-243009.00
ILE54	H	0.96	0.009	1.00	-320843.00

3.53.12 Detailed Probabilities of LYS53HD2:

Overall probability: 0.700

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS53	0.70	0.90

Expected NOESY Contacts

Proton	Expected probability
K53HA	0.98
K53HB2	1.00
K53HB3	1.00
K53HG2	1.00
K53HG3	1.00
K53HD3	1.00
K53HE2	1.00
K53HE3	1.00
K53HZ2	1.00
K53HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS53	HA	0.98	0.013	1.00	0.49
LYS53	HB2	1.00	0.209	0.00	0.00
LYS53	HB3	1.00	0.005	1.00	0.13
LYS53	HG2	1.00	0.004	1.00	0.28
LYS53	HG3	1.00	0.208	0.00	0.00
LYS53	HD2	1.00	0.211	0.00	0.00
LYS53	HD3	1.00	0.002	1.00	2.28
LYS53	HE2	1.00	0.004	1.00	0.22
LYS53	HE3	1.00	0.007	1.00	0.45
LYS53	H	0.88	0.015	1.00	-72527.00

3.53.13 Detailed Probabilities of LYS53HD3:

Overall probability: 0.902

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS53	0.90	0.90

Expected NOESY Contacts

Proton	Expected probability
K53HA	0.98
K53HB2	1.00
K53HB3	1.00
K53HG2	1.00
K53HG3	1.00
K53HD2	1.00
K53HE2	1.00
K53HE3	1.00
K53HZ2	1.00
K53HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS53	HA	0.98	0.076	0.02	0.00
LYS53	HB2	1.00	0.003	1.00	0.09
LYS53	HB3	1.00	0.001	1.00	0.16
LYS53	HG2	1.00	0.008	1.00	0.51
LYS53	HG3	1.00	0.014	1.00	0.56
LYS53	HD2	1.00	0.001	1.00	2.16
LYS53	HD3	1.00	0.002	1.00	6.06
LYS53	HE2	1.00	0.001	1.00	0.31
LYS53	HE3	1.00	0.002	1.00	0.50
LYS53	H	0.87	0.004	1.00	-119128.00

3.53.14 Detailed Probabilities of LYS53HE2:

Overall probability: 0.627

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS53	0.63	0.89

Expected NOESY Contacts

Proton	Expected probability
K53HB2	0.98
K53HB3	0.99
K53HG2	1.00
K53HG3	1.00
K53HD2	1.00
K53HD3	1.00
K53HE3	1.00
K53HZ2	1.00
K53HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS53	HB2	0.98	1.357	0.02	0.00
LYS53	HB3	0.99	0.010	1.00	0.08
LYS53	HG2	1.00	0.006	1.00	0.10
LYS53	HG3	1.00	0.940	0.00	0.00
LYS53	HD2	1.00	0.001	1.00	0.23
LYS53	HD3	1.00	0.016	1.00	0.25
LYS53	HE2	1.00	0.021	1.00	25.87
LYS53	HE3	1.00	0.078	0.00	0.00

3.53.15 Detailed Probabilities of LYS53HE3:

Overall probability: 0.378

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS53	0.38	0.89

Expected NOESY Contacts

Proton	Expected probability
K53HB2	0.99
K53HB3	0.99
K53HG2	1.00
K53HG3	1.00
K53HD2	1.00
K53HD3	1.00
K53HE2	1.00
K53HZ2	1.00
K53HE3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS53	HB2	0.99	1.446	0.01	0.00
LYS53	HB3	0.99	0.079	0.01	0.00
LYS53	HG2	1.00	0.001	1.00	0.07
LYS53	HG3	1.00	1.029	0.00	0.00
LYS53	HD2	1.00	0.090	0.00	0.00
LYS53	HD3	1.00	0.009	1.00	0.43
LYS53	HE2	1.00	0.068	0.00	0.00
LYS53	HE3	1.00	0.011	1.00	27.21

3.53.16 Detailed Probabilities of LYS53H:

Overall probability: 0.859

Overall confidence: 0.923

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU52	0.80	0.83
LYS53	0.86	1.00
ILE54	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E52HG2	0.98
E52HB2	1.00
E52H	1.00
E52HG3	0.96
E52HB3	1.00
E52HA	1.00
K53HA	1.00
K53HB2	1.00
K53HB3	1.00
K53HG2	1.00
K53HG3	1.00
K53H	1.00
I54H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU52	HA	1.00	0.009	1.00	0.75
GLU52	HB2	1.00	0.005	1.00	0.09
GLU52	HB3	1.00	0.011	1.00	0.10
GLU52	HG2	0.98	6.303	0.02	0.00
GLU52	HG3	0.96	0.001	1.00	0.07
LYS53	HA	1.00	0.017	1.00	0.36
LYS53	HB2	1.00	1.172	0.00	0.00
LYS53	HB3	1.00	0.011	1.00	0.12
LYS53	HG2	1.00	0.005	1.00	0.15
LYS53	HG3	1.00	0.006	1.00	0.11
LYS53	H	1.00	0.008	1.00	-5054351.00
LYS53	HD3	0.87	0.011	1.00	0.06
ILE54	H	1.00	0.009	1.00	-106715.00
ILE54	HA	0.93	0.027	1.00	0.24

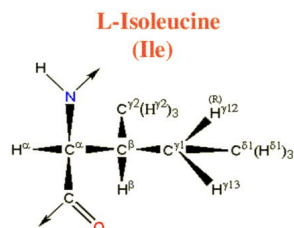


Figure 53: Image from the BMRB

Residue probability: 0.806
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	173.089	175.926	2.710	0.000	0.000
CA 3.54.1	59.264	61.717	4.152	0.545	1.000
CB 3.54.2	41.953	38.702	3.945	1.000	1.000
CG1 3.54.3	27.420	27.785	2.037	1.000	1.000
CG2 3.54.4	17.835	17.574	1.928	0.667	1.000
CD1 3.54.5	13.410	13.545	3.646	0.857	1.000
N 3.54.6	124.730	121.467	6.098	0.938	1.000
HA 3.54.7	4.846	4.185	1.403	0.900	1.000
HB 3.54.8	1.681	1.776	0.310	0.889	1.000
HG12 3.54.9	1.249	1.271	0.411	0.752	1.000
HG13 3.54.10	0.911	1.186	0.426	0.571	1.000
HG2 3.54.11	0.746	0.762	0.283	0.778	1.000
HD1 3.54.12	0.635	0.668	0.293	0.858	1.000
H 3.54.13	8.804	8.301	0.685	0.719	1.000

3.54.1 Detailed Probabilities of ILE54CA:

Overall probability: 0.545
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS53	0.50	1.00
ILE54	0.57	1.00
LEU55	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K53HA	1.00
I54HB	1.00
I54HG12	1.00
I54HG13	1.00
I54HG21	1.00
I54HD11	0.97
I54H	1.00
I54HA	1.00
L55H	1.00
L55HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS53	HA	1.00	0.059	0.00	0.00
LYS53	H	0.93	0.027	1.00	0.24
ILE54	HA	1.00	0.017	1.00	0.70
ILE54	HB	1.00	0.014	1.00	0.48
ILE54	HG12	1.00	0.060	0.00	0.00
ILE54	HG13	1.00	0.045	0.00	0.00
ILE54	HG21	1.00	0.011	1.00	0.08
ILE54	HD11	0.97	0.012	1.00	0.35
ILE54	H	1.00	0.083	0.00	0.00
LEU55	HA	1.00	0.019	1.00	0.23
LEU55	H	1.00	0.073	0.00	0.00

3.54.2 Detailed Probabilities of ILE54CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE54	1.00	1.00
LEU55	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I54HA	1.00
I54HG12	1.00
I54HG13	1.00
I54HG21	1.00
I54HD11	1.00
I54H	1.00
I54HB	1.00
L55H	1.00

NOESY contacts detailed probability

3.54 ILE(54)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE54	HA	1.00	0.006	1.00	0.20
ILE54	HB	1.00	0.010	1.00	4.56
ILE54	HG12	1.00	0.004	1.00	0.39
ILE54	HG13	1.00	0.000	1.00	0.52
ILE54	HG21	1.00	0.003	1.00	1.24
ILE54	HD11	1.00	0.016	1.00	1.23
ILE54	H	1.00	0.003	1.00	0.36
LEU55	H	1.00	0.001	1.00	0.11

3.54.3 Detailed Probabilities of ILE54CG1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE54	1.00	1.00
LEU55	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I54HA	1.00
I54HB	1.00
I54HG13	1.00
I54HG21	1.00
I54HD11	1.00
I54H	1.00
I54HG12	1.00
L55H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE54	HA	1.00	0.007	1.00	0.18
ILE54	HB	1.00	0.003	1.00	0.46
ILE54	HG12	1.00	0.001	1.00	5.04
ILE54	HG13	1.00	0.002	1.00	1.40
ILE54	HG21	1.00	0.003	1.00	2.11
ILE54	HD11	1.00	0.012	1.00	0.96
ILE54	H	1.00	0.005	1.00	0.14
LEU55	H	0.98	0.021	1.00	0.13

3.54.4 Detailed Probabilities of ILE54CG2:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE54	0.57	1.00
LEU55	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I54HA	1.00
I54HB	1.00
I54HG12	1.00
I54HG13	1.00
I54HG22	1.00
I54HD11	0.99
I54H	1.00
L55H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE54	HA	1.00	0.014	1.00	0.64
ILE54	HB	1.00	0.005	1.00	1.45
ILE54	HG12	1.00	0.009	1.00	0.52
ILE54	HG13	1.00	0.165	0.00	0.00
ILE54	HG21	1.00	0.330	0.00	0.00
ILE54	HD11	0.99	0.420	0.01	0.00
ILE54	H	1.00	0.012	1.00	0.44
LEU55	H	0.98	0.009	1.00	0.71
LEU55	HA	0.69	0.000	1.00	0.09

3.54.5 Detailed Probabilities of ILE54CD1:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE54	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
I54HA	0.97
I54HB	1.00
I54HG12	1.00
I54HG13	1.00
I54HG21	0.99
I54HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE54	HA	0.97	0.010	1.00	0.55
ILE54	HB	1.00	0.009	1.00	1.71
ILE54	HG12	1.00	0.008	1.00	1.29
ILE54	HG13	1.00	0.054	0.00	0.00
ILE54	HG21	0.99	0.008	1.00	10.40
ILE54	HD11	1.00	0.012	1.00	90.84
ILE54	H	0.94	0.013	1.00	0.59

3.54.6 Detailed Probabilities of ILE54N:

Overall probability: 0.938

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS53	0.88	1.00
ILE54	1.00	1.00
LEU55	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K53H	1.00
K53HG2	0.97
K53HG3	0.96
K53HA	1.00
K53HB2	1.00
K53HB3	1.00
I54HA	1.00
I54HB	1.00
I54HG12	1.00
I54HG13	1.00
I54HG21	1.00
I54H	1.00
L55H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS53	HA	1.00	0.006	1.00	-912658.00
LYS53	HB2	1.00	0.007	1.00	-93311.00
LYS53	HB3	1.00	0.044	0.00	0.00
LYS53	HG2	0.97	0.001	1.00	-170001.00
LYS53	HG3	0.96	0.009	1.00	-320843.00
LYS53	H	1.00	0.009	1.00	-106715.00
LYS53	HD2	0.54	0.026	1.00	-144797.00
LYS53	HD3	0.55	0.010	1.00	-254061.00
ILE54	HA	1.00	0.003	1.00	-251509.00
ILE54	HB	1.00	0.004	1.00	-585702.00
ILE54	HG12	1.00	0.009	1.00	-254061.00
ILE54	HG13	1.00	0.015	1.00	-320843.00
ILE54	HG21	1.00	0.001	1.00	-298060.00
ILE54	H	1.00	0.003	1.00	-3443142.00
ILE54	HD11	0.94	0.010	1.00	-364481.00
LEU55	H	1.00	0.000	1.00	-115318.00

3.54.7 Detailed Probabilities of ILE54HA:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS53	1.00	1.00
ILE54	1.00	1.00
LEU55	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K53HA	1.00
I54HB	1.00
I54HG12	1.00
I54HG13	1.00
I54HG21	1.00
I54HD11	0.97
I54H	1.00
I54HA	1.00
L55H	1.00
L55HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS53	HA	1.00	0.011	1.00	0.42
ILE54	HA	1.00	0.017	1.00	0.70
ILE54	HB	1.00	0.006	1.00	0.20
ILE54	HG12	1.00	0.007	1.00	0.18
ILE54	HG13	1.00	0.009	1.00	0.16
ILE54	HG21	1.00	0.014	1.00	0.64
ILE54	HD11	0.97	0.010	1.00	0.55
ILE54	H	1.00	0.003	1.00	-251509.00
LEU55	HA	1.00	0.216	0.00	0.00
LEU55	H	1.00	0.011	1.00	-1206557.00

3.54.8 Detailed Probabilities of ILE54HB:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE54	1.00	1.00
LEU55	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
I54HA	1.00
I54HG12	1.00
I54HG13	1.00
I54HG21	1.00
I54HD11	1.00
I54H	1.00
I54HB	1.00
L55H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE54	HA	1.00	0.014	1.00	0.48
ILE54	HB	1.00	0.010	1.00	4.56
ILE54	HG12	1.00	0.003	1.00	0.46
ILE54	HG13	1.00	0.002	1.00	0.34
ILE54	HG21	1.00	0.005	1.00	1.45
ILE54	HD11	1.00	0.009	1.00	1.71
ILE54	H	1.00	0.004	1.00	-585702.00
LEU55	H	1.00	0.089	0.00	0.00
LEU55	HA	0.89	0.025	1.00	0.27

3.54.9 Detailed Probabilities of ILE54HG12:

Overall probability: 0.752

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE54	0.86	1.00
LEU55	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
I54HA	1.00
I54HB	1.00
I54HG13	1.00
I54HG21	1.00
I54HD11	1.00
I54H	1.00
I54HG12	1.00
L55H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE54	HA	1.00	0.060	0.00	0.00
ILE54	HB	1.00	0.004	1.00	0.39
ILE54	HG12	1.00	0.001	1.00	5.04
ILE54	HG13	1.00	0.009	1.00	1.17
ILE54	HG21	1.00	0.009	1.00	0.52
ILE54	HD11	1.00	0.008	1.00	1.29
ILE54	H	1.00	0.009	1.00	-254061.00
LEU55	H	0.98	0.073	0.02	0.00

3.54.10 Detailed Probabilities of ILE54HG13:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE54	0.57	1.00

Expected NOESY Contacts

Proton	Expected probability
I54HA	1.00
I54HB	1.00
I54HG12	1.00
I54HG21	1.00
I54HD11	1.00
I54H	1.00
I54HG13	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE54	HA	1.00	0.045	0.00	0.00
ILE54	HB	1.00	0.000	1.00	0.52
ILE54	HG12	1.00	0.002	1.00	1.40
ILE54	HG13	1.00	0.009	1.00	5.21
ILE54	HG21	1.00	0.165	0.00	0.00
ILE54	HD11	1.00	0.054	0.00	0.00
ILE54	H	1.00	0.015	1.00	-320843.00

3.54.11 Detailed Probabilities of ILE54HG21:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE54	0.71	1.00
LEU55	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I54HA	1.00
I54HB	1.00
I54HG12	1.00
I54HG13	1.00
I54HG22	1.00
I54HD11	0.99
I54H	1.00
L55H	0.98

NOESY contacts detailed probability

3.54 ILE(54)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE54	HA	1.00	0.011	1.00	0.08
ILE54	HB	1.00	0.003	1.00	1.24
ILE54	HG12	1.00	0.003	1.00	2.11
ILE54	HG13	1.00	0.088	0.00	0.00
ILE54	HG21	1.00	0.330	0.00	0.00
ILE54	HD11	0.99	0.008	1.00	10.40
ILE54	H	1.00	0.001	1.00	-298060.00
LEU55	H	0.98	0.001	1.00	-901958.00
LEU55	HA	0.69	0.025	1.00	0.12

3.54.12 Detailed Probabilities of ILE54HD11:

Overall probability: 0.858

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE54	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
I54HA	0.97
I54HB	1.00
I54HG12	1.00
I54HG13	1.00
I54HG21	0.99
I54HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE54	HA	0.97	0.012	1.00	0.35
ILE54	HB	1.00	0.016	1.00	1.23
ILE54	HG12	1.00	0.012	1.00	0.96
ILE54	HG13	1.00	0.023	1.00	0.91
ILE54	HG21	0.99	0.420	0.01	0.00
ILE54	HD11	1.00	0.012	1.00	90.84
ILE54	H	0.94	0.010	1.00	-364481.00

3.54.13 Detailed Probabilities of ILE54H:

Overall probability: 0.719

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS53	0.51	1.00
ILE54	0.86	1.00
LEU55	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K53H	1.00
K53HG2	0.97
K53HG3	0.96
K53HA	1.00
K53HB2	1.00
K53HB3	1.00
I54HA	1.00
I54HB	1.00
I54HG12	1.00
I54HG13	1.00
I54HG21	1.00
I54H	1.00
L55H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS53	HA	1.00	0.017	1.00	0.35
LYS53	HB2	1.00	2.014	0.00	0.00
LYS53	HB3	1.00	0.021	1.00	0.06
LYS53	HG2	0.97	0.837	0.03	0.00
LYS53	HG3	0.96	0.510	0.04	0.00
LYS53	H	1.00	0.003	1.00	-137837.00
ILE54	HA	1.00	0.083	0.00	0.00
ILE54	HB	1.00	0.003	1.00	0.36
ILE54	HG12	1.00	0.005	1.00	0.14
ILE54	HG13	1.00	0.003	1.00	0.14
ILE54	HG21	1.00	0.012	1.00	0.44
ILE54	H	1.00	0.003	1.00	-3443142.00
ILE54	HD11	0.94	0.013	1.00	0.59
LEU55	H	1.00	0.015	1.00	-87351.00

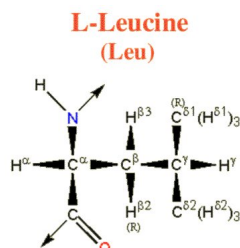
3.55 LEU(55)

Figure 54: Image from the BMRB

Residue probability: 0.696

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.430	177.056	1.929	0.000	0.000
CA 3.55.1	53.502	55.735	3.802	0.750	1.000
CB 3.55.2	45.202	42.389	3.750	0.844	1.000
CG 3.55.3	27.373	26.892	3.086	0.750	1.000
CD1 3.55.4	26.265	24.837	3.657	0.629	1.000
CD2 3.55.5	26.632	24.201	3.117	0.500	1.000
N 3.55.6	130.086	121.785	4.943	0.787	1.000
HA 3.55.7	5.641	4.315	0.840	0.909	1.000
HB2 3.55.8	1.761	1.601	0.373	0.625	1.000
HB3 3.55.9	1.320	1.508	0.398	0.750	1.000
HG 3.55.10	1.566	1.510	0.340	0.750	1.000
HD1 3.55.11	0.684	0.739	0.294	0.411	1.000
HD2 3.55.12	0.736	0.727	0.421	0.571	1.000
H 3.55.13	9.103	8.237	0.647	0.769	1.000

3.55.1 Detailed Probabilities of LEU55CA:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE54	0.67	1.00
LEU55	0.71	1.00
ILE56	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I54HA	1.00
L55HB2	1.00
L55HB3	1.00
L55HG	1.00
L55HD11	0.99
L55HD21	0.99
L55H	1.00
L55HA	1.00
I56H	1.00
I56HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE54	HA	1.00	0.216	0.00	0.00
ILE54	HB	0.89	0.025	1.00	0.27
ILE54	HG21	0.71	0.025	1.00	0.12
LEU55	HA	1.00	0.004	1.00	1.80
LEU55	HB2	1.00	0.105	0.00	0.00
LEU55	HB3	1.00	0.002	1.00	0.26
LEU55	HG	1.00	0.005	1.00	0.29
LEU55	HD11	0.99	0.023	1.00	0.48
LEU55	HD21	0.99	0.029	1.00	0.48
LEU55	H	1.00	0.083	0.00	0.00
ILE56	HA	1.00	0.005	1.00	0.06
ILE56	H	1.00	0.004	1.00	0.92

3.55.2 Detailed Probabilities of LEU55CB:

Overall probability: 0.844

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU55	0.94	1.00
ILE56	0.50	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
I56H	1.00

NOESY contacts detailed probability

3.55 LEU(55)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU55	HA	1.00	0.002	1.00	0.32
LEU55	HB2	1.00	0.005	1.00	1.39
LEU55	HB3	1.00	0.007	1.00	1.91
LEU55	HG	1.00	0.002	1.00	0.42
LEU55	HD11	1.00	0.034	0.60	0.00
LEU55	HD21	1.00	0.018	1.00	0.95
LEU55	H	1.00	0.003	1.00	0.29
ILE56	H	1.00	0.076	0.00	0.00
ILE56	HA	0.92	0.007	1.00	0.18

3.55.3 Detailed Probabilities of LEU55CG:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU55	0.71	1.00
ILE56	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
I56H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU55	HA	1.00	0.005	1.00	0.25
LEU55	HB2	1.00	0.030	1.00	0.00
LEU55	HB3	1.00	0.018	1.00	0.41
LEU55	HG	1.00	0.225	0.00	0.00
LEU55	HD11	1.00	0.051	0.00	0.00
LEU55	HD21	1.00	0.001	1.00	1.18
LEU55	H	1.00	0.000	1.00	0.11
ILE56	H	0.99	0.001	1.00	0.17

3.55.4 Detailed Probabilities of LEU55CD1:

Overall probability: 0.629

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU55	0.63	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	0.006	1.00	0.35
LEU55	HB2	1.00	0.001	1.00	0.52
LEU55	HB3	1.00	0.123	0.00	0.00
LEU55	HG	1.00	0.003	1.00	0.38
LEU55	HD11	1.00	0.036	0.40	0.00
LEU55	HD21	1.00	0.088	0.00	0.00
LEU55	H	0.86	0.016	1.00	0.29

3.55.5 Detailed Probabilities of LEU55CD2:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU55	0.50	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	0.004	1.00	0.20
LEU55	HB2	1.00	0.010	1.00	0.69
LEU55	HB3	1.00	0.003	1.00	0.57
LEU55	HG	1.00	0.205	0.00	0.00
LEU55	HD11	1.00	0.178	0.00	0.00
LEU55	HD21	1.00	0.126	0.00	0.00

3.55.6 Detailed Probabilities of LEU55N:

Overall probability: 0.787

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE54	0.67	1.00
LEU55	1.00	1.00
ILE56	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
I54HG21	0.98
I54HG12	0.98
I54HA	1.00
I54HB	1.00
I54H	1.00
L55HA	1.00
L55HB2	1.00
L55HB3	1.00
L55HG	1.00
L55H	1.00
I56H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE54	HA	1.00	0.011	1.00	-1206557.00
ILE54	HB	1.00	0.089	0.00	0.00
ILE54	HG12	0.98	0.073	0.02	0.00
ILE54	HG21	0.98	0.001	1.00	-901958.00
ILE54	H	1.00	0.015	1.00	-87351.00
ILE54	HG13	0.93	0.020	1.00	-248696.00
LEU55	HA	1.00	0.004	1.00	-287825.00
LEU55	HB2	1.00	0.009	1.00	-502799.00
LEU55	HB3	1.00	0.002	1.00	-312116.00
LEU55	HG	1.00	0.010	1.00	-112306.00
LEU55	H	1.00	0.005	1.00	-3307229.00
LEU55	HD21	0.87	0.011	1.00	-901958.00
ILE56	H	1.00	0.074	0.00	0.00
ILE56	HA	0.93	0.009	1.00	-338154.00

3.55.7 Detailed Probabilities of LEU55HA:

Overall probability: 0.909

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE54	1.00	1.00
LEU55	1.00	1.00
ILE56	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
I54HA	1.00
L55HB2	1.00
L55HB3	1.00
L55HG	1.00
L55HD11	0.99
L55HD21	0.99
L55H	1.00
L55HA	1.00
I56H	1.00
I56HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE54	HA	1.00	0.019	1.00	0.23
ILE54	HG21	0.71	0.000	1.00	0.09
LEU55	HA	1.00	0.004	1.00	1.80
LEU55	HB2	1.00	0.004	1.00	0.19
LEU55	HB3	1.00	0.002	1.00	0.32
LEU55	HG	1.00	0.005	1.00	0.25
LEU55	HD11	0.99	0.006	1.00	0.35
LEU55	HD21	0.99	0.004	1.00	0.20
LEU55	H	1.00	0.004	1.00	-287825.00
ILE56	HA	1.00	0.086	0.00	0.00
ILE56	H	1.00	0.003	1.00	-1346666.00

3.55.8 Detailed Probabilities of LEU55HB2:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU55	0.71	1.00
ILE56	0.00	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
I56H	1.00

NOESY contacts detailed probability

3.55 LEU(55)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU55	HA	1.00	0.105	0.00	0.00
LEU55	HB2	1.00	0.186	0.00	0.00
LEU55	HB3	1.00	0.005	1.00	1.39
LEU55	HG	1.00	0.030	1.00	0.00
LEU55	HD11	1.00	0.001	1.00	0.52
LEU55	HD21	1.00	0.010	1.00	0.69
LEU55	H	1.00	0.009	1.00	-502799.00
ILE56	H	1.00	0.077	0.00	0.00

3.55.9 Detailed Probabilities of LEU55HB3:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU55	0.71	1.00
ILE56	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
I56H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU55	HA	1.00	0.002	1.00	0.26
LEU55	HB2	1.00	0.229	0.00	0.00
LEU55	HB3	1.00	0.007	1.00	1.91
LEU55	HG	1.00	0.018	1.00	0.41
LEU55	HD11	1.00	0.123	0.00	0.00
LEU55	HD21	1.00	0.003	1.00	0.57
LEU55	H	1.00	0.002	1.00	-312116.00
ILE56	H	1.00	0.003	1.00	-160110.00

3.55.10 Detailed Probabilities of LEU55HG:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU55	0.71	1.00
ILE56	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
I56H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU55	HA	1.00	0.005	1.00	0.29
LEU55	HB2	1.00	0.009	1.00	0.31
LEU55	HB3	1.00	0.002	1.00	0.42
LEU55	HG	1.00	0.225	0.00	0.00
LEU55	HD11	1.00	0.003	1.00	0.38
LEU55	HD21	1.00	0.205	0.00	0.00
LEU55	H	1.00	0.010	1.00	-112306.00
ILE56	H	0.99	0.005	1.00	-340607.00

3.55.11 Detailed Probabilities of LEU55HD11:

Overall probability: 0.411

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU55	0.41	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	0.023	1.00	0.48
LEU55	HB2	1.00	0.204	0.00	0.00
LEU55	HB3	1.00	0.034	0.60	0.00
LEU55	HG	1.00	0.051	0.00	0.00
LEU55	HD11	1.00	0.036	0.40	0.00
LEU55	HD21	1.00	0.178	0.00	0.00
LEU55	H	0.88	0.034	0.88	0.00

3.55.12 Detailed Probabilities of LEU55HD21:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU55	0.57	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	0.029	1.00	0.48
LEU55	HB2	1.00	0.152	0.00	0.00
LEU55	HB3	1.00	0.018	1.00	0.95
LEU55	HG	1.00	0.001	1.00	1.18
LEU55	HD11	1.00	0.088	0.00	0.00
LEU55	HD21	1.00	0.126	0.00	0.00
LEU55	H	0.85	0.011	1.00	-901958.00

3.55.13 Detailed Probabilities of LEU55H:

Overall probability: 0.769

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE54	0.83	1.00
LEU55	0.83	1.00
ILE56	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I54HG21	0.98
I54HG12	0.98
I54HA	1.00
I54HB	1.00
I54H	1.00
L55HA	1.00
L55HB2	1.00
L55HB3	1.00
L55HG	1.00
L55H	1.00
I56H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE54	HA	1.00	0.073	0.00	0.00
ILE54	HB	1.00	0.001	1.00	0.11
ILE54	HG12	0.98	0.021	1.00	0.13
ILE54	HG21	0.98	0.009	1.00	0.71
ILE54	H	1.00	0.000	1.00	-115318.00
ILE54	HG13	0.93	0.003	1.00	0.06
LEU55	HA	1.00	0.083	0.00	0.00
LEU55	HB2	1.00	0.008	1.00	0.29
LEU55	HB3	1.00	0.003	1.00	0.29
LEU55	HG	1.00	0.000	1.00	0.11
LEU55	H	1.00	0.005	1.00	-3307229.00
LEU55	HD11	0.88	0.016	1.00	0.29
ILE56	H	1.00	0.082	0.00	0.00

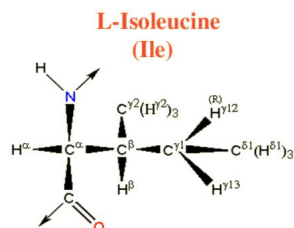


Figure 55: Image from the BMRB

Residue probability: 0.749
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.089	175.926	2.710	0.000	0.000
CA 3.56.1	59.110	61.717	4.152	0.692	1.000
CB 3.56.2	39.823	38.702	3.945	0.750	1.000
CG1 3.56.3	27.650	27.785	2.037	1.000	1.000
CG2 3.56.4	17.086	17.574	1.928	0.890	1.000
CD1 3.56.5	12.573	13.545	3.646	0.430	1.000
N 3.56.6	125.983	121.467	6.098	0.867	1.000
HA 3.56.7	5.057	4.185	1.403	0.938	1.000
HB 3.56.8	1.688	1.776	0.310	0.750	1.000
HG12 3.56.9	1.427	1.271	0.411	0.775	1.000
HG13 3.56.10	0.958	1.186	0.426	0.857	1.000
HG2 3.56.11	0.694	0.762	0.283	0.778	1.000
HD1 3.56.12	0.661	0.668	0.293	0.218	1.000
H 3.56.13	9.182	8.301	0.685	0.800	1.000

3.56.1 Detailed Probabilities of ILE56CA:

Overall probability: 0.692
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU55	0.00	1.00
ILE56	0.76	1.00
ILE57	0.75	1.00

Expected NOESY Contacts

Proton	Expected probability
L55HA	1.00
I56HB	1.00
I56HG12	1.00
I56HG13	1.00
I56HG21	1.00
I56HD11	0.97
I56H	1.00
I56HA	1.00
I57H	1.00
I57HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU55	HA	1.00	0.086	0.00	0.00
ILE56	HA	1.00	0.005	1.00	2.41
ILE56	HB	1.00	0.138	0.00	0.00
ILE56	HG12	1.00	0.025	1.00	0.28
ILE56	HG13	1.00	0.015	1.00	0.23
ILE56	HG21	1.00	0.004	1.00	0.89
ILE56	HD11	0.97	0.037	0.30	0.00
ILE56	H	1.00	0.029	1.00	0.25
ILE57	HA	1.00	0.150	0.00	0.00
ILE57	H	1.00	0.005	1.00	1.19
ILE57	HB	0.52	0.003	1.00	0.16
ILE57	HG12	0.51	0.008	1.00	0.28

3.56.2 Detailed Probabilities of ILE56CB:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE56	0.86	1.00
ILE57	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I56HA	1.00
I56HG12	1.00
I56HG13	1.00
I56HG21	1.00
I56HD11	1.00
I56H	1.00
I56HB	1.00
I57H	1.00

NOESY contacts detailed probability

3.56 ILE(56)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE56	HA	1.00	0.003	1.00	0.15
ILE56	HB	1.00	0.028	1.00	1.78
ILE56	HG12	1.00	0.015	1.00	0.43
ILE56	HG13	1.00	0.001	1.00	0.24
ILE56	HG21	1.00	0.007	1.00	1.82
ILE56	HD11	1.00	0.040	0.00	0.00
ILE56	H	1.00	0.000	1.00	0.40
ILE57	H	1.00	0.401	0.00	0.00

3.56.3 Detailed Probabilities of ILE56CG1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE56	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I56HA	1.00
I56HB	1.00
I56HG12	1.00
I56HG21	1.00
I56HD11	1.00
I56H	1.00
I56HG13	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE56	HA	1.00	0.002	1.00	0.28
ILE56	HB	1.00	0.005	1.00	0.54
ILE56	HG12	1.00	0.008	1.00	1.92
ILE56	HG13	1.00	0.001	1.00	3.17
ILE56	HG21	1.00	0.017	1.00	1.67
ILE56	HD11	1.00	0.016	1.00	1.67
ILE56	H	1.00	0.002	1.00	0.15

3.56.4 Detailed Probabilities of ILE56CG2:

Overall probability: 0.890

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE56	0.86	1.00
ILE57	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I56HA	1.00
I56HB	1.00
I56HG12	1.00
I56HG13	1.00
I56HG22	1.00
I56HD11	0.99
I56H	1.00
I57H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE56	HA	1.00	0.003	1.00	0.65
ILE56	HB	1.00	0.000	1.00	1.29
ILE56	HG12	1.00	0.016	1.00	0.76
ILE56	HG13	1.00	0.007	1.00	0.76
ILE56	HG21	1.00	0.009	1.00	37.91
ILE56	HD11	0.99	0.042	0.01	0.00
ILE56	H	1.00	0.003	1.00	0.17
ILE57	H	0.98	0.007	1.00	0.61
ILE57	HA	0.65	0.016	1.00	0.18

3.56.5 Detailed Probabilities of ILE56CD1:

Overall probability: 0.430

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE56	0.43	1.00

Expected NOESY Contacts

Proton	Expected probability
I56HA	0.97
I56HB	1.00
I56HG12	1.00
I56HG13	1.00
I56HG21	0.99
I56HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE56	HA	0.97	0.002	1.00	0.35
ILE56	HB	1.00	0.189	0.00	0.00
ILE56	HG12	1.00	0.009	1.00	1.40
ILE56	HG13	1.00	0.478	0.00	0.00
ILE56	HG21	0.99	0.742	0.01	0.00
ILE56	HD11	1.00	0.775	0.00	0.00
ILE56	H	0.94	0.015	1.00	0.21

3.56.6 Detailed Probabilities of ILE56N:

Overall probability: 0.867

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU55	0.71	1.00
ILE56	1.00	1.00
ILE57	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L55HB2	1.00
L55H	1.00
L55HB3	1.00
L55HA	1.00
L55HG	0.99
I56HA	1.00
I56HB	1.00
I56HG12	1.00
I56HG13	1.00
I56HG21	1.00
I56H	1.00
I57H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU55	HA	1.00	0.003	1.00	-1346666.00
LEU55	HB2	1.00	0.077	0.00	0.00
LEU55	HB3	1.00	0.003	1.00	-160110.00
LEU55	HG	0.99	0.005	1.00	-340607.00
LEU55	H	1.00	0.082	0.00	0.00
LEU55	HD11	0.53	0.025	1.00	-1119245.00
LEU55	HD21	0.63	0.027	1.00	-1119245.00
ILE56	HA	1.00	0.000	1.00	-270593.00
ILE56	HB	1.00	0.004	1.00	-740520.00
ILE56	HG12	1.00	0.015	1.00	-427733.00
ILE56	HG13	1.00	0.000	1.00	-186147.00
ILE56	HG21	1.00	0.015	1.00	-1119245.00
ILE56	H	1.00	0.003	1.00	-3855514.00
ILE57	H	1.00	0.005	1.00	-146079.00
ILE57	HG13	0.54	0.009	1.00	-209317.00

3.56.7 Detailed Probabilities of ILE56HA:

Overall probability: 0.938

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU55	1.00	1.00
ILE56	1.00	1.00
ILE57	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
L55HA	1.00
I56HB	1.00
I56HG12	1.00
I56HG13	1.00
I56HG21	1.00
I56HD11	0.97
I56H	1.00
I56HA	1.00
I57H	1.00
I57HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU55	HA	1.00	0.005	1.00	0.06
LEU55	HB2	0.60	0.006	1.00	0.18
LEU55	HB3	0.92	0.007	1.00	0.18
LEU55	H	0.93	0.009	1.00	-338154.00
ILE56	HA	1.00	0.005	1.00	2.41
ILE56	HB	1.00	0.003	1.00	0.15
ILE56	HG12	1.00	0.003	1.00	0.32
ILE56	HG13	1.00	0.002	1.00	0.28
ILE56	HG21	1.00	0.003	1.00	0.65
ILE56	HD11	0.97	0.002	1.00	0.35
ILE56	H	1.00	0.000	1.00	-270593.00
ILE57	HA	1.00	0.074	0.00	0.00
ILE57	H	1.00	0.004	1.00	-1863294.00
ILE57	HB	0.52	0.001	1.00	0.12
ILE57	HG12	0.51	0.003	1.00	0.32
ILE57	HG13	0.68	0.009	1.00	0.06

3.56.8 Detailed Probabilities of ILE56HB:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE56	0.71	1.00
ILE57	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I56HA	1.00
I56HG12	1.00
I56HG13	1.00
I56HG21	1.00
I56HD11	1.00
I56H	1.00
I56HB	1.00
I57H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE56	HA	1.00	0.138	0.00	0.00
ILE56	HB	1.00	0.028	1.00	1.78
ILE56	HG12	1.00	0.001	1.00	0.90
ILE56	HG13	1.00	0.005	1.00	0.54
ILE56	HG21	1.00	0.000	1.00	1.29
ILE56	HD11	1.00	0.189	0.00	0.00
ILE56	H	1.00	0.004	1.00	-740520.00
ILE57	H	1.00	0.005	1.00	-192772.00

3.56.9 Detailed Probabilities of ILE56HG12:

Overall probability: 0.775

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE56	0.86	1.00
ILE57	0.20	1.00

Expected NOESY Contacts

Proton	Expected probability
I56HA	1.00
I56HB	1.00
I56HG13	1.00
I56HG21	1.00
I56HD11	1.00
I56H	1.00
I56HG12	1.00
I57H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE56	HA	1.00	0.025	1.00	0.28
ILE56	HB	1.00	0.015	1.00	0.43
ILE56	HG12	1.00	0.228	0.00	0.00
ILE56	HG13	1.00	0.008	1.00	1.92
ILE56	HG21	1.00	0.016	1.00	0.76
ILE56	HD11	1.00	0.009	1.00	1.40
ILE56	H	1.00	0.015	1.00	-427733.00
ILE57	H	0.98	0.038	0.20	0.00

3.56.10 Detailed Probabilities of ILE56HG13:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE56	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
I56HA	1.00
I56HB	1.00
I56HG12	1.00
I56HG21	1.00
I56HD11	1.00
I56H	1.00
I56HG13	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE56	HA	1.00	0.015	1.00	0.23
ILE56	HB	1.00	0.001	1.00	0.24
ILE56	HG12	1.00	0.003	1.00	1.90
ILE56	HG13	1.00	0.001	1.00	3.17
ILE56	HG21	1.00	0.007	1.00	0.76
ILE56	HD11	1.00	0.478	0.00	0.00
ILE56	H	1.00	0.000	1.00	-186147.00

3.56.11 Detailed Probabilities of ILE56HG21:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE56	0.72	1.00
ILE57	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I56HA	1.00
I56HB	1.00
I56HG12	1.00
I56HG13	1.00
I56HG22	1.00
I56HD11	0.99
I56H	1.00
I57H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE56	HA	1.00	0.004	1.00	0.89
ILE56	HB	1.00	0.007	1.00	1.82
ILE56	HG12	1.00	0.261	0.00	0.00
ILE56	HG13	1.00	0.017	1.00	1.67
ILE56	HG21	1.00	0.009	1.00	37.91
ILE56	HD11	0.99	0.742	0.01	0.00
ILE56	H	1.00	0.015	1.00	-1119245.00
ILE57	H	0.98	0.007	1.00	-1612991.00
ILE57	HA	0.65	0.013	1.00	0.61

3.56.12 Detailed Probabilities of ILE56HD11:

Overall probability: 0.218

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE56	0.22	1.00

Expected NOESY Contacts

Proton	Expected probability
I56HA	0.97
I56HB	1.00
I56HG12	1.00
I56HG13	1.00
I56HG21	0.99
I56HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE56	HA	0.97	0.037	0.30	0.00
ILE56	HB	1.00	0.040	0.00	0.00
ILE56	HG12	1.00	0.294	0.00	0.00
ILE56	HG13	1.00	0.016	1.00	1.67
ILE56	HG21	0.99	0.042	0.01	0.00
ILE56	HD11	1.00	0.775	0.00	0.00

3.56.13 Detailed Probabilities of ILE56H:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU55	0.50	1.00
ILE56	1.00	1.00
ILE57	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L55HB2	1.00
L55H	1.00
L55HB3	1.00
L55HA	1.00
L55HG	0.99
I56HA	1.00
I56HB	1.00
I56HG12	1.00
I56HG13	1.00
I56HG21	1.00
I56H	1.00
I57H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU55	HA	1.00	0.004	1.00	0.92
LEU55	HB2	1.00	0.071	0.00	0.00
LEU55	HB3	1.00	0.076	0.00	0.00
LEU55	HG	0.99	0.001	1.00	0.17
LEU55	H	1.00	0.074	0.00	0.00
LEU55	HD11	0.53	0.014	1.00	0.14
ILE56	HA	1.00	0.029	1.00	0.25
ILE56	HB	1.00	0.000	1.00	0.40
ILE56	HG12	1.00	0.002	1.00	0.18
ILE56	HG13	1.00	0.002	1.00	0.15
ILE56	HG21	1.00	0.003	1.00	0.17
ILE56	H	1.00	0.003	1.00	-3855514.00
ILE56	HD11	0.94	0.015	1.00	0.21
ILE57	H	1.00	0.028	1.00	-239027.00
ILE57	HG13	0.54	0.025	1.00	0.05

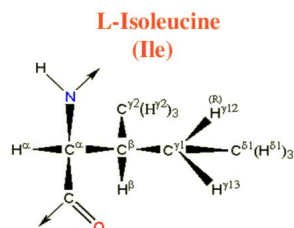


Figure 56: Image from the BMRB

Residue probability: 0.760
 Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.869	175.926	2.710	0.000	0.000
CA 3.57.1	59.255	61.717	4.152	0.636	1.000
CB 3.57.2	38.951	38.702	3.945	0.250	1.000
CG1 3.57.3	27.650	27.785	2.037	1.000	1.000
CG2 3.57.4	17.770	17.574	1.928	0.750	1.000
CD1 3.57.5	13.942	13.545	3.646	0.833	1.000
N 3.57.6	127.241	121.467	6.098	0.943	1.000
HA 3.57.7	4.912	4.185	1.403	0.818	1.000
HB 3.57.8	1.823	1.776	0.310	0.778	1.000
HG12 3.57.9	1.460	1.271	0.411	0.625	1.000
HG13 3.57.10	0.859	1.186	0.426	0.875	1.000
HG2 3.57.11	0.840	0.762	0.283	0.889	1.000
HD1 3.57.12	0.707	0.668	0.293	0.714	1.000
H 3.57.13	8.541	8.301	0.685	0.771	1.000

3.57.1 Detailed Probabilities of ILE57CA:

Overall probability: 0.636
 Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE56	0.50	1.00
ILE57	0.71	1.00
SER58	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
I56HA	1.00
I57HB	1.00
I57HG12	1.00
I57HG13	1.00
I57HG21	1.00
I57HD11	0.97
I57H	1.00
I57HA	1.00
S58HA	1.00
S58H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE56	HA	1.00	0.074	0.00	0.00
ILE56	HG21	0.68	0.013	1.00	0.61
ILE57	HA	1.00	0.001	1.00	2.01
ILE57	HB	1.00	0.009	1.00	0.43
ILE57	HG12	1.00	0.085	0.00	0.00
ILE57	HG13	1.00	0.012	1.00	0.48
ILE57	HG21	1.00	0.007	1.00	0.48
ILE57	HD11	0.97	0.000	1.00	0.61
ILE57	H	1.00	0.068	0.00	0.00
SER58	HA	1.00	0.096	0.00	0.00
SER58	H	1.00	0.010	1.00	0.81

3.57.2 Detailed Probabilities of ILE57CB:

Overall probability: 0.250

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE57	0.29	1.00
SER58	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I57HA	1.00
I57HG12	1.00
I57HG13	1.00
I57HG21	1.00
I57HD11	1.00
I57H	1.00
I57HB	1.00
S58H	1.00

NOESY contacts detailed probability

3.57 ILE(57)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE57	HA	1.00	0.005	1.00	0.13
ILE57	HB	1.00	0.643	0.00	0.00
ILE57	HG12	1.00	1.006	0.00	0.00
ILE57	HG13	1.00	1.607	0.00	0.00
ILE57	HG21	1.00	1.626	0.00	0.00
ILE57	HD11	1.00	1.759	0.00	0.00
ILE57	H	1.00	0.004	1.00	0.55
SER58	H	1.00	0.265	0.00	0.00

3.57.3 Detailed Probabilities of ILE57CG1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE57	1.00	1.00
SER58	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I57HA	1.00
I57HB	1.00
I57HG13	1.00
I57HG21	1.00
I57HD11	1.00
I57H	1.00
I57HG12	1.00
S58H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE57	HA	1.00	0.010	1.00	0.32
ILE57	HB	1.00	0.011	1.00	0.80
ILE57	HG12	1.00	0.001	1.00	12.32
ILE57	HG13	1.00	0.004	1.00	3.27
ILE57	HG21	1.00	0.015	1.00	3.27
ILE57	HD11	1.00	0.013	1.00	3.60
ILE57	H	1.00	0.005	1.00	0.39
SER58	H	0.98	0.006	1.00	0.18

3.57.4 Detailed Probabilities of ILE57CG2:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE57	0.71	1.00
SER58	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I57HA	1.00
I57HB	1.00
I57HG12	1.00
I57HG13	1.00
I57HG22	1.00
I57HD11	0.99
I57H	1.00
S58H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE57	HA	1.00	0.059	0.00	0.00
ILE57	HB	1.00	0.009	1.00	1.62
ILE57	HG12	1.00	0.135	0.00	0.00
ILE57	HG13	1.00	0.017	1.00	54.69
ILE57	HG21	1.00	0.002	1.00	54.69
ILE57	HD11	0.99	0.030	1.00	0.00
ILE57	H	1.00	0.008	1.00	0.30
SER58	H	0.98	0.002	1.00	0.75

3.57.5 Detailed Probabilities of ILE57CD1:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE57	0.83	1.00

Expected NOESY Contacts

Proton	Expected probability
I57HA	0.97
I57HB	1.00
I57HG12	1.00
I57HG13	1.00
I57HG21	0.99
I57HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE57	HA	0.97	0.008	1.00	0.34
ILE57	HB	1.00	0.007	1.00	1.33
ILE57	HG12	1.00	0.007	1.00	2.07
ILE57	HG13	1.00	0.014	1.00	8.32
ILE57	HG21	0.99	0.005	1.00	8.32
ILE57	HD11	1.00	0.138	0.00	0.00

3.57.6 Detailed Probabilities of ILE57N:

Overall probability: 0.943

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE56	0.87	1.00
ILE57	1.00	1.00
SER58	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I56H	1.00
I56HG22	0.98
I56HB	1.00
I56HG12	0.98
I56HA	1.00
I57HA	1.00
I57HB	1.00
I57HG12	1.00
I57HG13	1.00
I57HG21	1.00
I57H	1.00
S58H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE56	HA	1.00	0.004	1.00	-1863294.00
ILE56	HB	1.00	0.005	1.00	-192772.00
ILE56	HG12	0.98	0.038	0.20	0.00
ILE56	HG21	0.99	0.007	1.00	-1612991.00
ILE56	H	1.00	0.028	1.00	-239027.00
ILE56	HG13	0.92	0.003	1.00	-187167.00
ILE57	HA	1.00	0.009	1.00	-281142.00
ILE57	HB	1.00	0.007	1.00	-850741.00
ILE57	HG12	1.00	0.005	1.00	-548873.00
ILE57	HG13	1.00	0.014	1.00	-659891.00
ILE57	HG21	1.00	0.005	1.00	-659891.00
ILE57	H	1.00	0.004	1.00	-5001836.00
ILE57	HD11	0.94	0.006	1.00	-1612991.00
SER58	H	1.00	0.001	1.00	-114206.00

3.57.7 Detailed Probabilities of ILE57HA:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE56	0.50	1.00
ILE57	0.86	1.00
SER58	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I56HA	1.00
I57HB	1.00
I57HG12	1.00
I57HG13	1.00
I57HG21	1.00
I57HD11	0.97
I57H	1.00
I57HA	1.00
S58HA	1.00
S58H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE56	HA	1.00	0.150	0.00	0.00
ILE56	HG21	0.68	0.016	1.00	0.18
ILE57	HA	1.00	0.001	1.00	2.01
ILE57	HB	1.00	0.005	1.00	0.13
ILE57	HG12	1.00	0.010	1.00	0.32
ILE57	HG13	1.00	0.004	1.00	0.19
ILE57	HG21	1.00	0.059	0.00	0.00
ILE57	HD11	0.97	0.008	1.00	0.34
ILE57	H	1.00	0.009	1.00	-281142.00
SER58	HA	1.00	0.002	1.00	0.19
SER58	H	1.00	0.001	1.00	-1503738.00

3.57.8 Detailed Probabilities of ILE57HB:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE57	0.86	1.00
SER58	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
I57HA	1.00
I57HG12	1.00
I57HG13	1.00
I57HG21	1.00
I57HD11	1.00
I57H	1.00
I57HB	1.00
S58H	1.00

NOESY contacts detailed probability

3.57 ILE(57)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE57	HA	1.00	0.009	1.00	0.43
ILE57	HB	1.00	0.643	0.00	0.00
ILE57	HG12	1.00	0.011	1.00	0.80
ILE57	HG13	1.00	0.001	1.00	0.89
ILE57	HG21	1.00	0.009	1.00	1.62
ILE57	HD11	1.00	0.007	1.00	1.33
ILE57	H	1.00	0.007	1.00	-850741.00
SER58	H	1.00	0.067	0.00	0.00
SER58	HA	0.86	0.020	1.00	0.26

3.57.9 Detailed Probabilities of ILE57HG12:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE57	0.57	1.00
SER58	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I57HA	1.00
I57HB	1.00
I57HG13	1.00
I57HG21	1.00
I57HD11	1.00
I57H	1.00
I57HG12	1.00
S58H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE57	HA	1.00	0.085	0.00	0.00
ILE57	HB	1.00	1.006	0.00	0.00
ILE57	HG12	1.00	0.001	1.00	12.32
ILE57	HG13	1.00	0.006	1.00	1.99
ILE57	HG21	1.00	0.135	0.00	0.00
ILE57	HD11	1.00	0.007	1.00	2.07
ILE57	H	1.00	0.005	1.00	-548873.00
SER58	H	0.98	0.003	1.00	-167925.00

3.57.10 Detailed Probabilities of ILE57HG13:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE57	0.86	1.00
SER58	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I57HA	1.00
I57HB	1.00
I57HG12	1.00
I57HG21	1.00
I57HD11	1.00
I57H	1.00
I57HG13	1.00
S58H	0.95

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE57	HA	1.00	0.012	1.00	0.48
ILE57	HB	1.00	1.607	0.00	0.00
ILE57	HG12	1.00	0.004	1.00	3.27
ILE57	HG13	1.00	0.001	1.00	3.51
ILE57	HG21	1.00	0.017	1.00	54.69
ILE57	HD11	1.00	0.014	1.00	8.32
ILE57	H	1.00	0.014	1.00	-659891.00
SER58	H	0.95	0.018	1.00	-1141098.00

3.57.11 Detailed Probabilities of ILE57HG21:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE57	0.86	1.00
SER58	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I57HA	1.00
I57HB	1.00
I57HG12	1.00
I57HG13	1.00
I57HG22	1.00
I57HD11	0.99
I57H	1.00
S58H	0.98

NOESY contacts detailed probability

3.57 ILE(57)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE57	HA	1.00	0.007	1.00	0.48
ILE57	HB	1.00	1.626	0.00	0.00
ILE57	HG12	1.00	0.015	1.00	3.27
ILE57	HG13	1.00	0.018	1.00	3.51
ILE57	HG21	1.00	0.002	1.00	54.69
ILE57	HD11	0.99	0.005	1.00	8.32
ILE57	H	1.00	0.005	1.00	-659891.00
SER58	H	0.98	0.001	1.00	-1141098.00
SER58	HA	0.58	0.002	1.00	0.22

3.57.12 Detailed Probabilities of ILE57HD11:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE57	0.71	1.00

Expected NOESY Contacts

Proton	Expected probability
I57HA	0.97
I57HB	1.00
I57HG12	1.00
I57HG13	1.00
I57HG21	0.99
I57HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE57	HA	0.97	0.000	1.00	0.61
ILE57	HB	1.00	1.759	0.00	0.00
ILE57	HG12	1.00	0.013	1.00	3.60
ILE57	HG13	1.00	0.010	1.00	1.30
ILE57	HG21	0.99	0.030	1.00	0.00
ILE57	HD11	1.00	0.138	0.00	0.00
ILE57	H	0.94	0.006	1.00	-1612991.00

3.57.13 Detailed Probabilities of ILE57H:

Overall probability: 0.771

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE56	0.67	1.00
ILE57	0.83	1.00
SER58	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I56H	1.00
I56HG22	0.98
I56HB	1.00
I56HG12	0.98
I56HA	1.00
I57HA	1.00
I57HB	1.00
I57HG12	1.00
I57HG13	1.00
I57HG21	1.00
I57H	1.00
S58H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE56	HA	1.00	0.005	1.00	1.19
ILE56	HB	1.00	0.401	0.00	0.00
ILE56	HG12	0.98	0.135	0.02	0.00
ILE56	HG21	0.99	0.007	1.00	0.61
ILE56	H	1.00	0.005	1.00	-146079.00
ILE56	HG13	0.92	0.007	1.00	0.13
ILE57	HA	1.00	0.068	0.00	0.00
ILE57	HB	1.00	0.004	1.00	0.55
ILE57	HG12	1.00	0.005	1.00	0.39
ILE57	HG13	1.00	0.007	1.00	0.17
ILE57	HG21	1.00	0.008	1.00	0.30
ILE57	H	1.00	0.004	1.00	-5001836.00
SER58	H	1.00	0.007	1.00	-104139.00

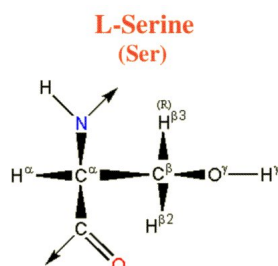


Figure 57: Image from the BMRB

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	174.211	174.682	1.868	0.000	0.000
CA 3.58.1	56.727	58.750	3.025	0.980	1.000
CB 3.58.2	66.615	63.523	4.288	1.000	1.000
N 3.58.3	119.270	116.135	5.326	0.815	1.000
HA 3.58.4	5.007	4.486	0.430	0.571	1.000
HB2 3.58.5	3.780	3.856	0.325	1.000	1.000
HB3 3.58.6	3.419	3.825	0.343	1.000	1.000
H 3.58.7	8.810	8.292	0.600	0.923	1.000
HG 3.58.8	5.092	5.146	1.319	0.960	1.000

3.58.1 Detailed Probabilities of SER58CA:

Overall probability: 0.980
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE57	1.00	1.00
SER58	0.96	1.00
ASN59	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I57HA	1.00
S58HB2	1.00
S58HB3	1.00
S58H	1.00
S58HG	1.00
S58HA	1.00
N59HA	1.00
N59H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE57	HA	1.00	0.002	1.00	0.19
ILE57	HB	0.86	0.020	1.00	0.26
ILE57	HG21	0.61	0.002	1.00	0.22
SER58	HA	1.00	0.004	1.00	3.48
SER58	HB2	1.00	0.006	1.00	0.49
SER58	HB3	1.00	0.003	1.00	0.54
SER58	H	1.00	0.008	1.00	1.15
SER58	HG	1.00	0.032	0.80	0.00
ASN59	HA	1.00	0.004	1.00	0.11
ASN59	H	1.00	0.008	1.00	1.15

3.58.2 Detailed Probabilities of SER58CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
SER58	1.00	1.00
ASN59	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S58HA	1.00
S58HB3	1.00
S58H	1.00
S58HG	1.00
S58HB2	1.00
N59H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER58	HA	1.00	0.002	1.00	0.43
SER58	HB2	1.00	0.003	1.00	1.31
SER58	HB3	1.00	0.008	1.00	1.47
SER58	H	1.00	0.004	1.00	0.32
SER58	HG	1.00	0.010	1.00	0.66
ASN59	H	1.00	0.012	1.00	0.32

3.58.3 Detailed Probabilities of SER58N:

Overall probability: 0.815

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE57	0.83	1.00
SER58	0.80	1.00
ASN59	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
I57H	1.00
I57HB	1.00
I57HG12	0.98
I57HG13	0.95
I57HA	1.00
I57HG22	0.98
S58HA	1.00
S58HB2	1.00
S58HB3	1.00
S58HG	1.00
S58H	1.00
N59H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE57	HA	1.00	0.001	1.00	-1503738.00
ILE57	HB	1.00	0.067	0.00	0.00
ILE57	HG12	0.98	0.003	1.00	-167925.00
ILE57	HG13	0.95	0.018	1.00	-1141098.00
ILE57	HG21	0.98	0.001	1.00	-1141098.00
ILE57	H	1.00	0.007	1.00	-104139.00
SER58	HA	1.00	0.087	0.00	0.00
SER58	HB2	1.00	0.000	1.00	-235200.00
SER58	HB3	1.00	0.008	1.00	-289274.00
SER58	H	1.00	0.018	1.00	-5590689.00
SER58	HG	1.00	0.002	1.00	-134217.00
ASN59	H	1.00	0.034	0.60	0.00
ASN59	HA	0.83	0.028	1.00	-96081.00

3.58.4 Detailed Probabilities of SER58HA:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE57	0.00	1.00
SER58	0.75	1.00
ASN59	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
I57HA	1.00
S58HB2	1.00
S58HB3	1.00
S58H	1.00
S58HG	1.00
S58HA	1.00
N59HA	1.00
N59H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE57	HA	1.00	0.096	0.00	0.00
SER58	HA	1.00	0.004	1.00	3.48
SER58	HB2	1.00	0.002	1.00	0.43
SER58	HB3	1.00	0.001	1.00	0.39
SER58	H	1.00	0.087	0.00	0.00
ASN59	HA	1.00	0.347	0.00	0.00
ASN59	H	1.00	0.006	1.00	-1689416.00

3.58.5 Detailed Probabilities of SER58HB2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
SER58	1.00	1.00
ASN59	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S58HA	1.00
S58HB3	1.00
S58H	1.00
S58HG	1.00
S58HB2	1.00
N59H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER58	HA	1.00	0.006	1.00	0.49
SER58	HB2	1.00	0.003	1.00	1.31
SER58	HB3	1.00	0.001	1.00	1.42
SER58	H	1.00	0.000	1.00	-235200.00
ASN59	H	1.00	0.001	1.00	-246639.00

3.58.6 Detailed Probabilities of SER58HB3:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
SER58	1.00	1.00
ASN59	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S58HA	1.00
S58HB2	1.00
S58H	1.00
S58HG	1.00
S58HB3	1.00
N59H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER58	HA	1.00	0.003	1.00	0.54
SER58	HB2	1.00	0.008	1.00	1.47
SER58	HB3	1.00	0.008	1.00	1.71
SER58	H	1.00	0.008	1.00	-289274.00
ASN59	H	1.00	0.003	1.00	-183102.00
ASN59	HA	0.71	0.018	1.00	0.25

3.58.7 Detailed Probabilities of SER58H:

Overall probability: 0.923

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE57	0.83	1.00
SER58	1.00	1.00
ASN59	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I57H	1.00
I57HB	1.00
I57HG12	0.98
I57HG13	0.95
I57HA	1.00
I57HG22	0.98
S58HA	1.00
S58HB2	1.00
S58HB3	1.00
S58HG	1.00
S58H	1.00
N59H	1.00

NOESY contacts detailed probability

3.58 SER(58)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE57	HA	1.00	0.010	1.00	0.81
ILE57	HB	1.00	0.265	0.00	0.00
ILE57	HG12	0.98	0.006	1.00	0.18
ILE57	HG13	0.95	0.017	1.00	0.09
ILE57	HG21	0.98	0.002	1.00	0.75
ILE57	H	1.00	0.001	1.00	-114206.00
SER58	HA	1.00	0.008	1.00	1.15
SER58	HB2	1.00	0.004	1.00	0.32
SER58	HB3	1.00	0.001	1.00	0.31
SER58	H	1.00	0.018	1.00	-5590689.00
ASN59	H	1.00	0.016	1.00	-5324546.00
ASN59	HA	0.83	0.019	1.00	1.06
ASN59	HB2	0.56	0.008	1.00	0.17

3.58.8 Detailed Probabilities of SER58HG:

Overall probability: 0.960

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
SER58	0.95	1.00
ASN59	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S58HA	1.00
S58HB2	1.00
S58HB3	1.00
S58H	1.00
N59H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER58	HA	1.00	0.032	0.80	0.00
SER58	HB2	1.00	0.010	1.00	0.66
SER58	HB3	1.00	0.009	1.00	0.54
SER58	H	1.00	0.002	1.00	-134217.00
ASN59	H	0.96	0.005	1.00	-344742.00

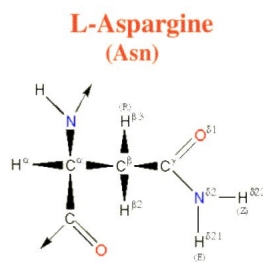
3.59 ASN(59)

Figure 58: Image from the BMRB

Residue probability: 0.817

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.795	175.315	1.862	0.000	0.000
CA 3.59.1	52.507	53.674	5.429	0.583	1.000
CB 3.59.2	38.962	38.785	5.449	0.875	1.000
N 3.59.3	122.382	118.907	6.480	0.919	1.000
ND2 3.59.4	109.566	112.932	14.355	1.000	1.000
HA 3.59.5	4.711	4.658	0.371	0.800	1.000
HB2 3.59.6	3.007	2.800	0.341	1.000	1.000
HB3 3.59.7	2.870	2.739	0.364	0.857	1.000
H 3.59.8	8.794	8.328	0.633	0.862	1.000
HD21 3.59.9	7.523	7.343	1.188	0.671	1.000
HD22 3.59.10	6.755	7.145	1.184	0.600	1.000

3.59.1 Detailed Probabilities of ASN59CA:

Overall probability: 0.583

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
SER58	0.67	1.00
ASN59	0.50	1.00
ASP60	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
S58HA	1.00
N59HB2	1.00
N59HB3	1.00
N59H	1.00
N59HD21	1.00
N59HD22	1.00
N59HA	1.00
D60HA	1.00
D60H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER58	HA	1.00	0.347	0.00	0.00
SER58	HB3	0.71	0.018	1.00	0.25
SER58	H	0.83	0.019	1.00	1.06
ASN59	HA	1.00	0.412	0.00	0.00
ASN59	HB2	1.00	0.010	1.00	1.03
ASN59	HB3	1.00	0.014	1.00	1.02
ASN59	H	1.00	0.003	1.00	1.06
ASN59	HD21	1.00	0.096	0.00	0.00
ASN59	HD22	1.00	0.101	0.00	0.00
ASP60	HA	1.00	0.011	1.00	0.37
ASP60	H	1.00	0.128	0.00	0.00
ASP60	HB2	0.53	0.008	1.00	0.67

3.59.2 Detailed Probabilities of ASN59CB:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN59	0.83	1.00
ASP60	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N59HA	1.00
N59HB2	1.00
N59H	1.00
N59HD21	1.00
N59HD22	1.00
N59HB3	1.00
D60H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN59	HA	1.00	0.005	1.00	0.49
ASN59	HB2	1.00	0.009	1.00	3.78
ASN59	HB3	1.00	0.128	0.00	0.00
ASN59	H	1.00	0.001	1.00	0.23
ASN59	HD21	1.00	0.005	1.00	0.30
ASN59	HD22	1.00	0.001	1.00	0.19
ASP60	H	1.00	0.008	1.00	0.05
ASP60	HA	0.75	0.018	1.00	0.09

3.59.3 Detailed Probabilities of ASN59N:

Overall probability: 0.919

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
SER58	1.00	1.00
ASN59	0.80	1.00
ASP60	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S58HB2	1.00
S58HA	1.00
S58HG	0.96
S58HB3	1.00
S58H	1.00
N59HA	1.00
N59HB2	1.00
N59HB3	1.00
N59HD21	0.98
N59H	1.00
D60H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER58	HA	1.00	0.006	1.00	-1689416.00
SER58	HB2	1.00	0.001	1.00	-246639.00
SER58	HB3	1.00	0.003	1.00	-183102.00
SER58	H	1.00	0.016	1.00	-5324546.00
SER58	HG	0.96	0.005	1.00	-344742.00
ASN59	HA	1.00	0.002	1.00	-375042.00
ASN59	HB2	1.00	0.005	1.00	-284313.00
ASN59	HB3	1.00	0.001	1.00	-395651.00
ASN59	H	1.00	0.000	1.00	-5324546.00
ASN59	HD21	0.98	0.337	0.02	0.00
ASP60	H	1.00	0.003	1.00	-916923.00
ASP60	HB2	0.57	0.010	1.00	-126188.00

3.59.4 Detailed Probabilities of ASN59ND2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN59	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N59HA	1.00
N59HB2	1.00
N59HB3	1.00
N59HD21	1.00
N59HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN59	HA	1.00	0.007	1.00	-91104.00
ASN59	HB2	1.00	0.006	1.00	-261156.00
ASN59	HB3	1.00	0.010	1.00	-458516.00
ASN59	HD21	1.00	0.001	1.00	-5675712.00
ASN59	HD22	1.00	0.003	1.00	-6608768.00

3.59.5 Detailed Probabilities of ASN59HA:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
SER58	1.00	1.00
ASN59	0.83	1.00
ASP60	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
S58HA	1.00
N59HB2	1.00
N59HB3	1.00
N59H	1.00
N59HD21	1.00
N59HD22	1.00
N59HA	1.00
D60HA	1.00
D60H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER58	HA	1.00	0.004	1.00	0.11
SER58	H	0.83	0.028	1.00	-96081.00
ASN59	HA	1.00	0.412	0.00	0.00
ASN59	HB2	1.00	0.010	1.00	0.64
ASN59	HB3	1.00	0.005	1.00	0.49
ASN59	H	1.00	0.002	1.00	-375042.00
ASN59	HD21	1.00	0.009	1.00	-154062.00
ASN59	HD22	1.00	0.007	1.00	-91104.00
ASP60	HA	1.00	0.144	0.00	0.00
ASP60	H	1.00	0.004	1.00	-298539.00

3.59.6 Detailed Probabilities of ASN59HB2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN59	1.00	1.00
ASP60	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N59HA	1.00
N59HB3	1.00
N59H	1.00
N59HD21	1.00
N59HD22	1.00
N59HB2	1.00
D60H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN59	HA	1.00	0.010	1.00	1.03
ASN59	HB2	1.00	0.013	1.00	4.05
ASN59	HB3	1.00	0.009	1.00	3.78
ASN59	H	1.00	0.005	1.00	-284313.00
ASN59	HD21	1.00	0.000	1.00	-364210.00
ASN59	HD22	1.00	0.006	1.00	-261156.00
ASP60	H	1.00	0.006	1.00	-100151.00
ASP60	HA	0.62	0.024	1.00	0.26

3.59.7 Detailed Probabilities of ASN59HB3:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN59	0.83	1.00
ASP60	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N59HA	1.00
N59HB2	1.00
N59H	1.00
N59HD21	1.00
N59HD22	1.00
N59HB3	1.00
D60H	1.00

NOESY contacts detailed probability

3.59 ASN(59)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN59	HA	1.00	0.014	1.00	1.02
ASN59	HB2	1.00	0.008	1.00	1.90
ASN59	HB3	1.00	0.128	0.00	0.00
ASN59	H	1.00	0.001	1.00	-395651.00
ASN59	HD21	1.00	0.008	1.00	-550588.00
ASN59	HD22	1.00	0.010	1.00	-458516.00
ASP60	H	1.00	0.002	1.00	-136976.00

3.59.8 Detailed Probabilities of ASN59H:

Overall probability: 0.862

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
SER58	0.90	1.00
ASN59	0.80	1.00
ASP60	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S58HB2	1.00
S58HA	1.00
S58HG	0.96
S58HB3	1.00
S58H	1.00
N59HA	1.00
N59HB2	1.00
N59HB3	1.00
N59HD21	0.98
N59H	1.00
D60H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER58	HA	1.00	0.008	1.00	1.15
SER58	HB2	1.00	0.012	1.00	0.32
SER58	HB3	1.00	0.015	1.00	0.31
SER58	H	1.00	0.034	0.60	0.00
ASN59	HA	1.00	0.003	1.00	1.06
ASN59	HB2	1.00	0.008	1.00	0.17
ASN59	HB3	1.00	0.001	1.00	0.23
ASN59	H	1.00	0.000	1.00	-5324546.00
ASN59	HD21	0.98	1.270	0.02	0.00
ASP60	H	1.00	0.002	1.00	-1037759.00

3.59.9 Detailed Probabilities of ASN59HD21:

Overall probability: 0.671

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN59	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
N59HA	1.00
N59HB2	1.00
N59HB3	1.00
N59H	0.98
N59HD22	1.00
N59HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN59	HA	1.00	0.096	0.00	0.00
ASN59	HB2	1.00	0.003	1.00	0.19
ASN59	HB3	1.00	0.005	1.00	0.30
ASN59	H	0.98	0.337	0.02	0.00
ASN59	HD21	1.00	0.001	1.00	-6604754.00
ASN59	HD22	1.00	0.001	1.00	-5675712.00

3.59.10 Detailed Probabilities of ASN59HD22:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN59	0.60	1.00

Expected NOESY Contacts

Proton	Expected probability
N59HA	1.00
N59HB2	1.00
N59HB3	1.00
N59HD21	1.00
N59HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN59	HA	1.00	0.101	0.00	0.00
ASN59	HB2	1.00	0.275	0.00	0.00
ASN59	HB3	1.00	0.001	1.00	0.19
ASN59	HD21	1.00	0.002	1.00	-5863932.00
ASN59	HD22	1.00	0.003	1.00	-6608768.00

3.60 ASP(60)

Figure 59: Image from the BMRB

Residue probability: 0.732

Residue probability confidence: 0.893

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	176.015	176.463	2.348	0.000	0.000
CA 3.60.1	53.097	54.786	4.266	0.525	0.875
CB 3.60.2	42.949	40.949	3.070	0.800	0.833
N 3.60.3	119.744	120.550	5.690	1.000	1.000
HD2	NA	—	—	0.000	0.000
HA 3.60.4	4.863	4.587	0.329	0.778	0.875
HB2 3.60.5	2.735	2.708	0.282	0.600	0.833
HB3 3.60.6	2.568	2.654	0.285	0.640	0.833
H 3.60.7	7.857	8.304	1.027	0.778	1.000

3.60.1 Detailed Probabilities of ASP60CA:

Overall probability: 0.525

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN59	0.50	1.00
ASP60	0.55	0.80
LYS61	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
N59HA	1.00
D60HD2	1.00
D60HB2	1.00
D60HB3	1.00
D60H	1.00
D60HA	1.00
K61H	1.00
K61HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN59	HA	1.00	0.144	0.00	0.00
ASN59	HB2	0.62	0.024	1.00	0.26
ASP60	HA	1.00	0.010	1.00	2.35
ASP60	HB2	1.00	0.045	0.00	0.00
ASP60	HB3	1.00	0.038	0.20	0.00
ASP60	H	1.00	0.013	1.00	0.33
LYS61	HA	1.00	0.234	0.00	0.00
LYS61	H	1.00	0.002	1.00	0.77

3.60.2 Detailed Probabilities of ASP60CB:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP60	0.75	0.80
LYS61	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D60HD2	1.00
D60HA	1.00
D60HB2	1.00
D60H	1.00
D60HB3	1.00
K61H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP60	HA	1.00	0.005	1.00	0.33
ASP60	HB2	1.00	0.006	1.00	1.43
ASP60	HB3	1.00	0.173	0.00	0.00
ASP60	H	1.00	0.004	1.00	0.29
LYS61	H	1.00	0.002	1.00	0.09

3.60.3 Detailed Probabilities of ASP60N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN59	1.00	1.00
ASP60	1.00	1.00
LYS61	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N59HB3	1.00
N59HB2	1.00
N59HA	1.00
N59H	1.00
D60HA	1.00
D60HB2	1.00
D60HB3	1.00
D60H	1.00
K61H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN59	HA	1.00	0.004	1.00	-298539.00
ASN59	HB2	1.00	0.006	1.00	-100151.00
ASN59	HB3	1.00	0.002	1.00	-136976.00
ASN59	H	1.00	0.002	1.00	-1037759.00
ASP60	HA	1.00	0.006	1.00	-430293.00
ASP60	HB2	1.00	0.004	1.00	-636718.00
ASP60	HB3	1.00	0.007	1.00	-642269.00
ASP60	H	1.00	0.005	1.00	-8391413.00
LYS61	H	1.00	0.005	1.00	-78303.00

3.60.4 Detailed Probabilities of ASP60HA:

Overall probability: 0.778

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN59	1.00	1.00
ASP60	0.75	0.80
LYS61	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
N59HA	1.00
D60HD2	1.00
D60HB2	1.00
D60HB3	1.00
D60H	1.00
D60HA	1.00
K61H	1.00
K61HA	1.00

NOESY contacts detailed probability

3.60 ASP(60)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN59	HA	1.00	0.011	1.00	0.37
ASN59	HB2	0.62	0.007	1.00	0.05
ASN59	HB3	0.75	0.018	1.00	0.09
ASP60	HA	1.00	0.010	1.00	2.35
ASP60	HB2	1.00	2.283	0.00	0.00
ASP60	HB3	1.00	0.005	1.00	0.33
ASP60	H	1.00	0.006	1.00	-430293.00
LYS61	HA	1.00	0.793	0.00	0.00
LYS61	H	1.00	0.013	1.00	-1169051.00

3.60.5 Detailed Probabilities of ASP60HB2:

Overall probability: 0.600

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP60	0.50	0.80
LYS61	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D60HD2	1.00
D60HA	1.00
D60HB3	1.00
D60H	1.00
D60HB2	1.00
K61H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP60	HA	1.00	0.045	0.00	0.00
ASP60	HB2	1.00	0.155	0.00	0.00
ASP60	HB3	1.00	0.006	1.00	1.43
ASP60	H	1.00	0.004	1.00	-636718.00
LYS61	H	1.00	0.007	1.00	-117207.00

3.60.6 Detailed Probabilities of ASP60HB3:

Overall probability: 0.640

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP60	0.55	0.80
LYS61	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D60HD2	1.00
D60HA	1.00
D60HB2	1.00
D60H	1.00
D60HB3	1.00
K61H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP60	HA	1.00	0.038	0.20	0.00
ASP60	HB2	1.00	0.012	1.00	1.22
ASP60	HB3	1.00	0.173	0.00	0.00
ASP60	H	1.00	0.007	1.00	-642269.00
LYS61	H	1.00	0.012	1.00	-159358.00

3.60.7 Detailed Probabilities of ASP60H:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN59	0.50	1.00
ASP60	1.00	1.00
LYS61	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N59HB3	1.00
N59HB2	1.00
N59HA	1.00
N59H	1.00
D60HA	1.00
D60HB2	1.00
D60HB3	1.00
D60H	1.00
K61H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN59	HA	1.00	0.128	0.00	0.00
ASN59	HB2	1.00	0.213	0.00	0.00
ASN59	HB3	1.00	0.008	1.00	0.05
ASN59	H	1.00	0.003	1.00	-916923.00
ASP60	HA	1.00	0.013	1.00	0.33
ASP60	HB2	1.00	0.005	1.00	0.25
ASP60	HB3	1.00	0.004	1.00	0.29
ASP60	H	1.00	0.005	1.00	-8391413.00
LYS61	H	1.00	0.006	1.00	-86244.00

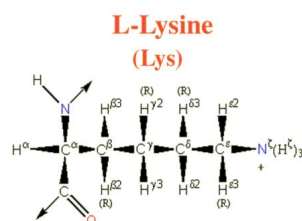


Figure 60: Image from the BMRB

Residue probability: 0.762
Residue probability confidence: 0.945

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	177.673	176.660	3.133	0.000	0.000
CA 3.61.1	59.632	57.014	3.028	0.775	1.000
CB 3.61.2	31.518	32.981	3.186	0.755	1.000
CG 3.61.3	24.910	24.941	1.956	0.818	0.917
CD 3.61.4	28.780	29.020	2.193	0.778	0.900
CE 3.61.5	41.780	41.893	1.492	0.627	0.889
N 3.61.6	125.818	120.954	4.210	1.000	1.000
NZ	NA	—	—	0.000	0.000
HA 3.61.7	3.722	4.262	0.489	0.873	1.000
HB2 3.61.8	1.517	1.774	0.365	0.818	1.000
HB3 3.61.9	1.432	1.742	0.385	0.729	1.000
HG2 3.61.10	1.029	1.358	0.344	0.545	0.917
HG3 3.61.11	1.257	1.343	0.357	0.727	0.917
HD2 3.61.12	1.173	1.614	0.957	0.444	0.900
HD3 3.61.13	1.096	1.595	0.387	0.579	0.900
HE2 3.61.14	2.686	2.907	0.230	0.937	0.889
HE3 3.61.15	2.674	2.901	0.241	0.877	0.889
H 3.61.16	8.904	8.185	0.605	0.917	1.000
HZ	NA	—	—	0.000	0.000

3.61.1 Detailed Probabilities of LYS61CA:

Overall probability: 0.775
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP60	0.00	1.00
LYS61	0.88	1.00
GLN62	0.75	1.00

Expected NOESY Contacts

Proton	Expected probability
D60HA	1.00
K61HB2	1.00
K61HB3	1.00
K61HG2	1.00
K61HG3	1.00
K61HD2	0.98
K61HD3	0.98
K61H	1.00
K61HA	1.00
Q62H	1.00
Q62HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP60	HA	1.00	0.793	0.00	0.00
LYS61	HA	1.00	0.000	1.00	3.93
LYS61	HB2	1.00	0.002	1.00	0.49
LYS61	HB3	1.00	0.006	1.00	0.49
LYS61	HG2	1.00	0.001	1.00	0.32
LYS61	HG3	1.00	0.010	1.00	0.28
LYS61	HD2	0.98	0.025	1.00	0.11
LYS61	HD3	0.98	0.052	0.02	0.00
LYS61	H	1.00	0.005	1.00	0.25
GLN62	HA	1.00	0.035	0.50	0.00
GLN62	H	1.00	0.011	1.00	0.15

3.61.2 Detailed Probabilities of LYS61CB:

Overall probability: 0.755

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS61	0.83	1.00
GLN62	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K61HA	1.00
K61HB3	1.00
K61HG2	1.00
K61HG3	1.00
K61HD2	1.00
K61HD3	1.00
K61HE2	0.98
K61HE3	0.99
K61H	1.00
K61HB2	1.00
Q62H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS61	HA	1.00	0.005	1.00	0.32
LYS61	HB2	1.00	0.002	1.00	1.35
LYS61	HB3	1.00	0.005	1.00	1.09
LYS61	HG2	1.00	0.010	1.00	0.29
LYS61	HG3	1.00	0.013	1.00	0.34
LYS61	HD2	1.00	0.040	0.00	0.00
LYS61	HD3	1.00	0.037	0.30	0.00
LYS61	HE2	0.98	0.010	1.00	0.06
LYS61	HE3	0.99	0.002	1.00	0.06
LYS61	H	1.00	0.001	1.00	0.17
GLN62	H	1.00	0.471	0.00	0.00

3.61.3 Detailed Probabilities of LYS61CG:

Overall probability: 0.818

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS61	0.80	0.91
GLN62	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K61HA	1.00
K61HB2	1.00
K61HB3	1.00
K61HG3	1.00
K61HD2	1.00
K61HD3	1.00
K61HE2	1.00
K61HE3	1.00
K61H	1.00
K61HZ2	1.00
K61HG2	1.00
Q62H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS61	HA	1.00	0.003	1.00	0.15
LYS61	HB2	1.00	0.024	1.00	0.41
LYS61	HB3	1.00	0.024	1.00	0.32
LYS61	HG2	1.00	0.128	0.00	0.00
LYS61	HG3	1.00	0.009	1.00	1.12
LYS61	HD2	1.00	0.016	1.00	0.65
LYS61	HD3	1.00	0.061	0.00	0.00
LYS61	HE2	1.00	0.001	1.00	0.16
LYS61	HE3	1.00	0.011	1.00	0.16
LYS61	H	1.00	0.014	1.00	0.14
GLN62	H	0.97	0.006	1.00	0.08

3.61.4 Detailed Probabilities of LYS61CD:

Overall probability: 0.778

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS61	0.78	0.90

Expected NOESY Contacts

Proton	Expected probability
K61HA	0.98
K61HB2	1.00
K61HB3	1.00
K61HG2	1.00
K61HG3	1.00
K61HD3	1.00
K61HE2	1.00
K61HE3	1.00
K61HZ2	1.00
K61HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS61	HA	0.98	0.010	1.00	0.14
LYS61	HB2	1.00	0.013	1.00	0.23
LYS61	HB3	1.00	0.007	1.00	0.26
LYS61	HG2	1.00	0.068	0.00	0.00
LYS61	HG3	1.00	0.084	0.00	0.00
LYS61	HD2	1.00	0.000	1.00	3.04
LYS61	HD3	1.00	0.001	1.00	2.37
LYS61	HE2	1.00	0.002	1.00	0.38
LYS61	HE3	1.00	0.010	1.00	0.38

3.61.5 Detailed Probabilities of LYS61CE:

Overall probability: 0.627

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS61	0.63	0.89

Expected NOESY Contacts

Proton	Expected probability
K61HB2	0.99
K61HB3	0.99
K61HG2	1.00
K61HG3	1.00
K61HD2	1.00
K61HD3	1.00
K61HE2	1.00
K61HZ2	1.00
K61HE3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS61	HB2	0.99	0.030	1.00	0.45
LYS61	HB3	0.99	0.163	0.01	0.00
LYS61	HG2	1.00	0.064	0.00	0.00
LYS61	HG3	1.00	0.010	1.00	0.31
LYS61	HD2	1.00	0.073	0.00	0.00
LYS61	HD3	1.00	0.002	1.00	0.59
LYS61	HE2	1.00	0.020	1.00	27.21
LYS61	HE3	1.00	0.025	1.00	25.87

3.61.6 Detailed Probabilities of LYS61N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP60	1.00	1.00
LYS61	1.00	1.00
GLN62	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D60HA	1.00
D60H	1.00
D60HB2	1.00
D60HB3	1.00
K61HA	1.00
K61HB2	1.00
K61HB3	1.00
K61HG2	1.00
K61HG3	1.00
K61H	1.00
Q62H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP60	HA	1.00	0.013	1.00	-1169051.00
ASP60	HB2	1.00	0.007	1.00	-117207.00
ASP60	HB3	1.00	0.012	1.00	-159358.00
ASP60	H	1.00	0.006	1.00	-86244.00
LYS61	HA	1.00	0.000	1.00	-366524.00
LYS61	HB2	1.00	0.001	1.00	-432079.00
LYS61	HB3	1.00	0.009	1.00	-363092.00
LYS61	HG2	1.00	0.001	1.00	-340699.00
LYS61	HG3	1.00	0.011	1.00	-373648.00
LYS61	H	1.00	0.001	1.00	-2480544.00
GLN62	H	1.00	0.009	1.00	-492626.00

3.61.7 Detailed Probabilities of LYS61HA:

Overall probability: 0.873

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP60	0.00	1.00
LYS61	1.00	1.00
GLN62	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
D60HA	1.00
K61HB2	1.00
K61HB3	1.00
K61HG2	1.00
K61HG3	1.00
K61HD2	0.98
K61HD3	0.98
K61H	1.00
K61HA	1.00
Q62H	1.00
Q62HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP60	HA	1.00	0.234	0.00	0.00
LYS61	HA	1.00	0.000	1.00	3.93
LYS61	HB2	1.00	0.005	1.00	0.32
LYS61	HB3	1.00	0.004	1.00	0.27
LYS61	HG2	1.00	0.003	1.00	0.15
LYS61	HG3	1.00	0.003	1.00	0.15
LYS61	HD2	0.98	0.010	1.00	0.14
LYS61	HD3	0.98	0.010	1.00	0.14
LYS61	H	1.00	0.000	1.00	-366524.00
GLN62	HA	1.00	0.034	0.60	0.00
GLN62	H	1.00	0.002	1.00	-202594.00

3.61.8 Detailed Probabilities of LYS61HB2:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS61	0.80	1.00
GLN62	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K61HA	1.00
K61HB3	1.00
K61HG2	1.00
K61HG3	1.00
K61HD2	1.00
K61HD3	1.00
K61HE2	0.98
K61HE3	0.99
K61H	1.00
K61HB2	1.00
Q62H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS61	HA	1.00	0.002	1.00	0.49
LYS61	HB2	1.00	0.002	1.00	1.35
LYS61	HB3	1.00	0.001	1.00	1.05
LYS61	HG2	1.00	0.024	1.00	0.41
LYS61	HG3	1.00	0.486	0.00	0.00
LYS61	HD2	1.00	0.013	1.00	0.23
LYS61	HD3	1.00	0.067	0.00	0.00
LYS61	HE2	0.98	0.030	1.00	0.45
LYS61	HE3	0.99	0.030	1.00	0.45
LYS61	H	1.00	0.001	1.00	-432079.00
GLN62	H	1.00	0.003	1.00	-227628.00

3.61.9 Detailed Probabilities of LYS61HB3:

Overall probability: 0.729

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS61	0.70	1.00
GLN62	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K61HA	1.00
K61HB2	1.00
K61HG2	1.00
K61HG3	1.00
K61HD2	1.00
K61HD3	1.00
K61HE2	0.99
K61HE3	0.99
K61H	1.00
K61HB3	1.00
Q62H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS61	HA	1.00	0.006	1.00	0.49
LYS61	HB2	1.00	0.005	1.00	1.09
LYS61	HB3	1.00	0.006	1.00	1.14
LYS61	HG2	1.00	0.024	1.00	0.32
LYS61	HG3	1.00	0.401	0.00	0.00
LYS61	HD2	1.00	0.007	1.00	0.26
LYS61	HD3	1.00	0.018	1.00	0.29
LYS61	HE2	0.99	0.163	0.01	0.00
LYS61	HE3	0.99	0.163	0.01	0.00
LYS61	H	1.00	0.009	1.00	-363092.00
GLN62	H	1.00	0.004	1.00	-216465.00

3.61.10 Detailed Probabilities of LYS61HG2:

Overall probability: 0.545

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS61	0.50	0.91
GLN62	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K61HA	1.00
K61HB2	1.00
K61HB3	1.00
K61HG3	1.00
K61HD2	1.00
K61HD3	1.00
K61HE2	1.00
K61HE3	1.00
K61H	1.00
K61HZ2	1.00
K61HG2	1.00
Q62H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS61	HA	1.00	0.001	1.00	0.32
LYS61	HB2	1.00	0.010	1.00	0.29
LYS61	HB3	1.00	0.009	1.00	0.28
LYS61	HG2	1.00	0.128	0.00	0.00
LYS61	HG3	1.00	0.002	1.00	1.06
LYS61	HD2	1.00	0.068	0.00	0.00
LYS61	HD3	1.00	0.066	0.00	0.00
LYS61	HE2	1.00	0.064	0.00	0.00
LYS61	HE3	1.00	0.064	0.00	0.00
LYS61	H	1.00	0.001	1.00	-340699.00
GLN62	H	0.97	0.004	1.00	-160991.00

3.61.11 Detailed Probabilities of LYS61HG3:

Overall probability: 0.727

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS61	0.70	0.91
GLN62	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K61HA	1.00
K61HB2	1.00
K61HB3	1.00
K61HG2	1.00
K61HD2	1.00
K61HD3	1.00
K61HE2	1.00
K61HE3	1.00
K61H	1.00
K61HZ2	1.00
K61HG3	1.00
Q62H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS61	HA	1.00	0.010	1.00	0.28
LYS61	HB2	1.00	0.013	1.00	0.34
LYS61	HB3	1.00	0.008	1.00	0.31
LYS61	HG2	1.00	0.009	1.00	1.12
LYS61	HG3	1.00	0.226	0.00	0.00
LYS61	HD2	1.00	0.084	0.00	0.00
LYS61	HD3	1.00	0.096	0.00	0.00
LYS61	HE2	1.00	0.010	1.00	0.31
LYS61	HE3	1.00	0.010	1.00	0.31
LYS61	H	1.00	0.011	1.00	-373648.00
GLN62	H	0.96	0.007	1.00	-94767.00

3.61.12 Detailed Probabilities of LYS61HD2:

Overall probability: 0.444

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS61	0.44	0.90

Expected NOESY Contacts

Proton	Expected probability
K61HA	0.98
K61HB2	1.00
K61HB3	1.00
K61HG2	1.00
K61HG3	1.00
K61HD3	1.00
K61HE2	1.00
K61HE3	1.00
K61HZ2	1.00
K61HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS61	HA	0.98	0.025	1.00	0.11
LYS61	HB2	1.00	0.040	0.00	0.00
LYS61	HB3	1.00	0.043	0.00	0.00
LYS61	HG2	1.00	0.016	1.00	0.65
LYS61	HG3	1.00	0.142	0.00	0.00
LYS61	HD2	1.00	0.000	1.00	3.04
LYS61	HD3	1.00	0.012	1.00	2.61
LYS61	HE2	1.00	0.073	0.00	0.00
LYS61	HE3	1.00	0.073	0.00	0.00

3.61.13 Detailed Probabilities of LYS61HD3:

Overall probability: 0.579

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS61	0.58	0.90

Expected NOESY Contacts

Proton	Expected probability
K61HA	0.98
K61HB2	1.00
K61HB3	1.00
K61HG2	1.00
K61HG3	1.00
K61HD2	1.00
K61HE2	1.00
K61HE3	1.00
K61HZ2	1.00
K61HD3	1.00

NOESY contacts detailed probability

3.61 LYS(61)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS61	HA	0.98	0.052	0.02	0.00
LYS61	HB2	1.00	0.037	0.30	0.00
LYS61	HB3	1.00	0.034	0.60	0.00
LYS61	HG2	1.00	0.061	0.00	0.00
LYS61	HG3	1.00	0.065	0.00	0.00
LYS61	HD2	1.00	0.001	1.00	2.37
LYS61	HD3	1.00	0.001	1.00	3.32
LYS61	HE2	1.00	0.002	1.00	0.59
LYS61	HE3	1.00	0.002	1.00	0.59
LYS61	H	0.87	0.034	0.87	0.00

3.61.14 Detailed Probabilities of LYS61HE2:

Overall probability: 0.937

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS61	0.94	0.89

Expected NOESY Contacts

Proton	Expected probability
K61HB2	0.98
K61HB3	0.99
K61HG2	1.00
K61HG3	1.00
K61HD2	1.00
K61HD3	1.00
K61HE3	1.00
K61HZ2	1.00
K61HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS61	HB2	0.98	0.010	1.00	0.06
LYS61	HB3	0.99	0.035	0.50	0.00
LYS61	HG2	1.00	0.001	1.00	0.16
LYS61	HG3	1.00	0.002	1.00	0.15
LYS61	HD2	1.00	0.002	1.00	0.38
LYS61	HD3	1.00	0.002	1.00	0.37
LYS61	HE2	1.00	0.020	1.00	27.21
LYS61	HE3	1.00	0.020	1.00	27.21

3.61.15 Detailed Probabilities of LYS61HE3:

Overall probability: 0.877

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS61	0.88	0.89

Expected NOESY Contacts

Proton	Expected probability
K61HB2	0.99
K61HB3	0.99
K61HG2	1.00
K61HG3	1.00
K61HD2	1.00
K61HD3	1.00
K61HE2	1.00
K61HZ2	1.00
K61HE3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS61	HB2	0.99	0.002	1.00	0.06
LYS61	HB3	0.99	0.047	0.01	0.00
LYS61	HG2	1.00	0.011	1.00	0.16
LYS61	HG3	1.00	0.014	1.00	0.15
LYS61	HD2	1.00	0.010	1.00	0.38
LYS61	HD3	1.00	0.010	1.00	0.37
LYS61	HE2	1.00	0.025	1.00	25.87
LYS61	HE3	1.00	0.025	1.00	25.87

3.61.16 Detailed Probabilities of LYS61H:

Overall probability: 0.917

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP60	0.75	1.00
LYS61	1.00	1.00
GLN62	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D60HA	1.00
D60H	1.00
D60HB2	1.00
D60HB3	1.00
K61HA	1.00
K61HB2	1.00
K61HB3	1.00
K61HG2	1.00
K61HG3	1.00
K61H	1.00
Q62H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP60	HA	1.00	0.002	1.00	0.77
ASP60	HB2	1.00	1.042	0.00	0.00
ASP60	HB3	1.00	0.002	1.00	0.09
ASP60	H	1.00	0.005	1.00	-78303.00
LYS61	HA	1.00	0.005	1.00	0.25
LYS61	HB2	1.00	0.001	1.00	0.17
LYS61	HB3	1.00	0.003	1.00	0.16
LYS61	HG2	1.00	0.014	1.00	0.14
LYS61	HG3	1.00	0.008	1.00	0.13
LYS61	H	1.00	0.001	1.00	-2480544.00
LYS61	HD3	0.87	0.000	1.00	0.05
GLN62	H	1.00	0.001	1.00	-400602.00

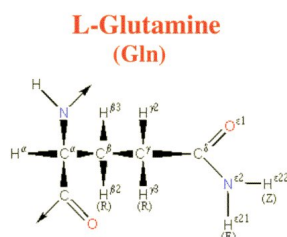


Figure 61: Image from the BMRB

Residue probability: 0.870
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.747	176.405	1.998	0.000	0.000
CA 3.62.1	58.301	56.667	2.318	0.700	1.000
CB 3.62.2	27.448	29.436	2.799	0.667	1.000
CG 3.62.3	33.720	33.781	1.871	1.000	1.000
N 3.62.4	118.918	119.799	3.762	1.000	1.000
NE2 3.62.5	112.559	111.924	2.434	1.000	1.000
HA 3.62.6	4.105	4.265	0.455	0.688	1.000
HB 3.62.7	2.167	2.047	0.290	1.000	1.000
HG2 3.62.8	2.413	2.308	0.289	1.000	1.000
HG3 3.62.9	2.412	2.284	0.313	1.000	1.000
H 3.62.10	8.434	8.232	0.711	0.788	1.000
HE21 3.62.11	7.847	7.217	0.496	0.800	1.000
HE22 3.62.12	6.890	7.041	0.463	0.800	1.000

3.62.1 Detailed Probabilities of GLN62CA:

Overall probability: 0.700
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS61	0.60	1.00
GLN62	0.80	1.00
LEU63	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K61HA	1.00
Q62HB2	1.00
Q62HG2	1.00
Q62HG3	1.00
Q62H	1.00
Q62HA	1.00
L63H	1.00
L63HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS61	HA	1.00	0.034	0.60	0.00
GLN62	HA	1.00	0.289	0.00	0.00
GLN62	HB2	1.00	0.009	1.00	1.89
GLN62	HG2	1.00	0.009	1.00	0.81
GLN62	HG3	1.00	0.010	1.00	0.81
GLN62	H	1.00	0.006	1.00	0.71
LEU63	HA	1.00	0.318	0.00	0.00
LEU63	H	1.00	0.000	1.00	0.52

3.62.2 Detailed Probabilities of GLN62CB:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN62	0.57	1.00
LEU63	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q62HA	1.00
Q62HB3	1.00
Q62HG2	1.00
Q62HG3	1.00
Q62H	1.00
Q62HE21	1.00
Q62HE22	1.00
L63H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN62	HA	1.00	0.003	1.00	0.94
GLN62	HB2	1.00	0.006	1.00	7.79
GLN62	HG2	1.00	0.006	1.00	1.60
GLN62	HG3	1.00	0.007	1.00	1.60
GLN62	H	1.00	0.766	0.00	0.00
GLN62	HE21	1.00	0.179	0.00	0.00
GLN62	HE22	1.00	0.778	0.00	0.00
LEU63	H	1.00	0.003	1.00	0.33
LEU63	HA	0.87	0.026	1.00	0.94

3.62.3 Detailed Probabilities of GLN62CG:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN62	1.00	1.00
LEU63	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q62HA	1.00
Q62HB2	1.00
Q62HG3	1.00
Q62H	1.00
Q62HE21	1.00
Q62HE22	1.00
Q62HG2	1.00
L63H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN62	HA	1.00	0.029	1.00	1.02
GLN62	HB2	1.00	0.023	1.00	4.31
GLN62	HG2	1.00	0.003	1.00	103.18
GLN62	HG3	1.00	0.004	1.00	103.18
GLN62	H	1.00	0.003	1.00	0.54
GLN62	HE21	1.00	0.004	1.00	0.44
GLN62	HE22	1.00	0.006	1.00	0.45
LEU63	H	0.97	0.006	1.00	0.08

3.62.4 Detailed Probabilities of GLN62N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS61	1.00	1.00
GLN62	1.00	1.00
LEU63	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K61H	1.00
K61HG3	0.96
K61HG2	0.97
K61HB3	1.00
K61HA	1.00
K61HB2	1.00
Q62HA	1.00
Q62HB2	1.00
Q62HG2	1.00
Q62HG3	1.00
Q62H	1.00
L63H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS61	HA	1.00	0.002	1.00	-202594.00
LYS61	HB2	1.00	0.003	1.00	-227628.00
LYS61	HB3	1.00	0.004	1.00	-216465.00
LYS61	HG2	0.97	0.004	1.00	-160991.00
LYS61	HG3	0.96	0.007	1.00	-94767.00
LYS61	H	1.00	0.001	1.00	-400602.00
GLN62	HA	1.00	0.003	1.00	-827116.00
GLN62	HB2	1.00	0.006	1.00	-1891321.00
GLN62	HG2	1.00	0.009	1.00	-798454.00
GLN62	HG3	1.00	0.010	1.00	-798454.00
GLN62	H	1.00	0.007	1.00	-9347159.00
LEU63	H	1.00	0.001	1.00	-1691796.00
LEU63	HA	0.94	0.026	1.00	-827116.00
LEU63	HB2	0.64	0.002	1.00	-129592.00

3.62.5 Detailed Probabilities of GLN62NE2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN62	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q62HB2	1.00
Q62HG2	1.00
Q62HG3	1.00
Q62HE22	1.00
Q62HE21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN62	HB2	1.00	0.011	1.00	-175559.00
GLN62	HG2	1.00	0.012	1.00	-946741.00
GLN62	HG3	1.00	0.013	1.00	-946741.00
GLN62	HE21	1.00	0.011	1.00	-25813160.00
GLN62	HE22	1.00	0.001	1.00	-10909495.00

3.62.6 Detailed Probabilities of GLN62HA:

Overall probability: 0.688

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS61	0.50	1.00
GLN62	0.80	1.00
LEU63	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K61HA	1.00
Q62HB2	1.00
Q62HG2	1.00
Q62HG3	1.00
Q62H	1.00
Q62HA	1.00
L63H	1.00
L63HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS61	HA	1.00	0.035	0.50	0.00
GLN62	HA	1.00	0.289	0.00	0.00
GLN62	HB2	1.00	0.003	1.00	0.94
GLN62	HG2	1.00	0.029	1.00	1.02
GLN62	HG3	1.00	0.029	1.00	1.02
GLN62	H	1.00	0.003	1.00	-827116.00
LEU63	HA	1.00	0.166	0.00	0.00
LEU63	H	1.00	0.016	1.00	-770813.00

3.62.7 Detailed Probabilities of GLN62HB2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN62	1.00	1.00
LEU63	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q62HA	1.00
Q62HB3	1.00
Q62HG2	1.00
Q62HG3	1.00
Q62H	1.00
Q62HE21	1.00
Q62HE22	1.00
L63H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN62	HA	1.00	0.009	1.00	1.89
GLN62	HB2	1.00	0.006	1.00	7.79
GLN62	HG2	1.00	0.023	1.00	4.31
GLN62	HG3	1.00	0.023	1.00	4.31
GLN62	H	1.00	0.006	1.00	-1891321.00
GLN62	HE21	1.00	0.011	1.00	-175559.00
GLN62	HE22	1.00	0.016	1.00	-91097.00
LEU63	H	1.00	0.006	1.00	-624135.00

3.62.8 Detailed Probabilities of GLN62HG2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN62	1.00	1.00
LEU63	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q62HA	1.00
Q62HB2	1.00
Q62HG3	1.00
Q62H	1.00
Q62HE21	1.00
Q62HE22	1.00
Q62HG2	1.00
L63H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN62	HA	1.00	0.010	1.00	0.81
GLN62	HB2	1.00	0.007	1.00	1.60
GLN62	HG2	1.00	0.004	1.00	103.18
GLN62	HG3	1.00	0.004	1.00	103.18
GLN62	H	1.00	0.010	1.00	-798454.00
GLN62	HE21	1.00	0.013	1.00	-946741.00
GLN62	HE22	1.00	0.005	1.00	-510518.00
LEU63	H	0.97	0.016	1.00	-136141.00

3.62.9 Detailed Probabilities of GLN62HG3:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN62	1.00	1.00
LEU63	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q62HA	1.00
Q62HB2	1.00
Q62HG2	1.00
Q62H	1.00
Q62HE21	1.00
Q62HE22	1.00
Q62HG3	1.00
L63H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN62	HA	1.00	0.010	1.00	0.81
GLN62	HB2	1.00	0.007	1.00	1.60
GLN62	HG2	1.00	0.004	1.00	103.18
GLN62	HG3	1.00	0.004	1.00	103.18
GLN62	H	1.00	0.010	1.00	-798454.00
GLN62	HE21	1.00	0.013	1.00	-946741.00
GLN62	HE22	1.00	0.005	1.00	-510518.00
LEU63	H	0.97	0.016	1.00	-136141.00

3.62.10 Detailed Probabilities of GLN62H:

Overall probability: 0.788

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS61	0.67	1.00
GLN62	0.80	1.00
LEU63	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K61H	1.00
K61HG3	0.96
K61HG2	0.97
K61HB3	1.00
K61HA	1.00
K61HB2	1.00
Q62HA	1.00
Q62HB2	1.00
Q62HG2	1.00
Q62HG3	1.00
Q62H	1.00
L63H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS61	HA	1.00	0.011	1.00	0.15
LYS61	HB2	1.00	0.471	0.00	0.00
LYS61	HB3	1.00	0.001	1.00	0.10
LYS61	HG2	0.97	0.006	1.00	0.08
LYS61	HG3	0.96	0.478	0.04	0.00
LYS61	H	1.00	0.009	1.00	-492626.00
GLN62	HA	1.00	0.006	1.00	0.71
GLN62	HB2	1.00	0.766	0.00	0.00
GLN62	HG2	1.00	0.003	1.00	0.54
GLN62	HG3	1.00	0.003	1.00	0.54
GLN62	H	1.00	0.007	1.00	-9347159.00
LEU63	H	1.00	0.009	1.00	-1142792.00
LEU63	HA	0.94	0.007	1.00	0.16
LEU63	HB2	0.64	0.002	1.00	0.09

3.62.11 Detailed Probabilities of GLN62HE21:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN62	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
Q62HB2	1.00
Q62HG2	1.00
Q62HG3	1.00
Q62HE22	1.00
Q62HE21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN62	HB2	1.00	0.179	0.00	0.00
GLN62	HG2	1.00	0.004	1.00	0.44
GLN62	HG3	1.00	0.004	1.00	0.44
GLN62	HE21	1.00	0.011	1.00	-25813160.00
GLN62	HE22	1.00	0.012	1.00	-13577290.00

3.62.12 Detailed Probabilities of GLN62HE22:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN62	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
Q62HB2	1.00
Q62HG2	1.00
Q62HG3	1.00
Q62HE21	1.00
Q62HE22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN62	HB2	1.00	0.778	0.00	0.00
GLN62	HG2	1.00	0.006	1.00	0.45
GLN62	HG3	1.00	0.006	1.00	0.45
GLN62	HE21	1.00	0.001	1.00	-10909495.00
GLN62	HE22	1.00	0.002	1.00	-31513908.00

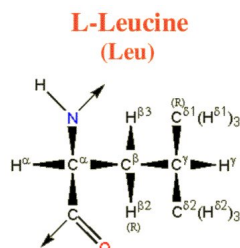
3.63 LEU(63)

Figure 62: Image from the BMRB

Residue probability: 0.693

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.552	177.056	1.929	0.000	0.000
CA 3.63.1	56.643	55.735	3.802	0.437	1.000
CB 3.63.2	40.894	42.389	3.750	0.988	1.000
CG 3.63.3	26.770	26.892	3.086	0.752	1.000
CD1 3.63.4	25.212	24.837	3.657	0.833	1.000
CD2 3.63.5	22.932	24.201	3.117	0.144	1.000
N 3.63.6	120.071	121.785	4.943	0.923	1.000
HA 3.63.7	4.134	4.315	0.840	0.667	1.000
HB2 3.63.8	1.871	1.601	0.373	0.656	1.000
HB3 3.63.9	1.426	1.508	0.398	0.863	1.000
HG 3.63.10	1.620	1.510	0.340	0.750	1.000
HD1 3.63.11	0.741	0.739	0.294	0.572	1.000
HD2 3.63.12	0.709	0.727	0.421	0.573	1.000
H 3.63.13	7.671	8.237	0.647	0.857	1.000

3.63.1 Detailed Probabilities of LEU63CA:

Overall probability: 0.437

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN62	0.50	1.00
LEU63	0.43	1.00
LEU64	0.40	1.00

Expected NOESY Contacts

Proton	Expected probability
Q62HA	1.00
L63HB2	1.00
L63HB3	1.00
L63HG	1.00
L63HD11	0.99
L63HD21	0.99
L63H	1.00
L63HA	1.00
L64H	1.00
L64HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN62	HA	1.00	0.166	0.00	0.00
GLN62	H	0.94	0.007	1.00	0.16
LEU63	HA	1.00	0.195	0.00	0.00
LEU63	HB2	1.00	0.220	0.00	0.00
LEU63	HB3	1.00	0.006	1.00	0.79
LEU63	HG	1.00	0.008	1.00	0.41
LEU63	HD11	0.99	0.691	0.01	0.00
LEU63	HD21	0.99	0.723	0.01	0.00
LEU63	H	1.00	0.003	1.00	0.63
LEU64	HA	1.00	0.032	0.80	0.00
LEU64	H	1.00	0.042	0.00	0.00

3.63.2 Detailed Probabilities of LEU63CB:

Overall probability: 0.988

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU63	0.99	1.00
LEU64	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L63HA	1.00
L63HB2	1.00
L63HG	1.00
L63HD11	1.00
L63HD21	1.00
L63H	1.00
L63HB3	1.00
L64H	1.00

NOESY contacts detailed probability

3.63 LEU(63)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU63	HA	1.00	0.007	1.00	0.50
LEU63	HB2	1.00	0.001	1.00	1.81
LEU63	HB3	1.00	0.031	0.90	0.00
LEU63	HG	1.00	0.012	1.00	1.02
LEU63	HD11	1.00	0.015	1.00	1.16
LEU63	HD21	1.00	0.017	1.00	1.16
LEU63	H	1.00	0.029	1.00	0.66
LEU64	H	1.00	0.016	1.00	0.66

3.63.3 Detailed Probabilities of LEU63CG:

Overall probability: 0.752

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU63	0.86	1.00
LEU64	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
L63HA	1.00
L63HB2	1.00
L63HB3	1.00
L63HD11	1.00
L63HD21	1.00
L63H	1.00
L63HG	1.00
L64H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU63	HA	1.00	0.009	1.00	0.23
LEU63	HB2	1.00	0.023	1.00	1.00
LEU63	HB3	1.00	0.002	1.00	0.91
LEU63	HG	1.00	0.016	1.00	19.97
LEU63	HD11	1.00	0.006	1.00	1.18
LEU63	HD21	1.00	0.026	1.00	1.18
LEU63	H	1.00	0.555	0.00	0.00
LEU64	H	0.98	0.510	0.02	0.00

3.63.4 Detailed Probabilities of LEU63CD1:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU63	0.83	1.00

Expected NOESY Contacts

Proton	Expected probability
L63HA	0.99
L63HB2	1.00
L63HB3	1.00
L63HG	1.00
L63HD12	1.00
L63HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU63	HA	0.99	0.006	1.00	0.35
LEU63	HB2	1.00	0.017	1.00	2.66
LEU63	HB3	1.00	0.015	1.00	3.93
LEU63	HG	1.00	0.108	0.00	0.00
LEU63	HD11	1.00	0.014	1.00	164.25
LEU63	HD21	1.00	0.018	1.00	164.25

3.63.5 Detailed Probabilities of LEU63CD2:

Overall probability: 0.144

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU63	0.14	1.00

Expected NOESY Contacts

Proton	Expected probability
L63HA	0.99
L63HB2	1.00
L63HB3	1.00
L63HG	1.00
L63HD11	1.00
L63HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU63	HA	0.99	0.204	0.01	0.00
LEU63	HB2	1.00	0.258	0.00	0.00
LEU63	HB3	1.00	0.244	0.00	0.00
LEU63	HG	1.00	0.438	0.00	0.00
LEU63	HD11	1.00	0.129	0.00	0.00
LEU63	HD21	1.00	0.161	0.00	0.00
LEU63	H	0.85	0.024	1.00	0.42

3.63.6 Detailed Probabilities of LEU63N:

Overall probability: 0.923

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN62	1.00	1.00
LEU63	1.00	1.00
LEU64	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q62HG3	0.97
Q62HB3	1.00
Q62HA	1.00
Q62H	1.00
Q62HG2	0.98
L63HA	1.00
L63HB2	1.00
L63HB3	1.00
L63HG	1.00
L63H	1.00
L64H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN62	HA	1.00	0.016	1.00	-770813.00
GLN62	HB2	1.00	0.006	1.00	-624135.00
GLN62	HG2	0.98	0.015	1.00	-136141.00
GLN62	HG3	0.97	0.016	1.00	-136141.00
GLN62	H	1.00	0.009	1.00	-1142792.00
LEU63	HA	1.00	0.013	1.00	-770813.00
LEU63	HB2	1.00	0.003	1.00	-722484.00
LEU63	HB3	1.00	0.004	1.00	-549172.00
LEU63	HG	1.00	0.007	1.00	-975670.00
LEU63	H	1.00	0.001	1.00	-6075660.00
LEU63	HD11	0.88	0.014	1.00	-554866.00
LEU63	HD21	0.87	0.018	1.00	-554866.00
LEU64	H	1.00	0.044	0.00	0.00

3.63.7 Detailed Probabilities of LEU63HA:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN62	0.67	1.00
LEU63	0.72	1.00
LEU64	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
Q62HA	1.00
L63HB2	1.00
L63HB3	1.00
L63HG	1.00
L63HD11	0.99
L63HD21	0.99
L63H	1.00
L63HA	1.00
L64H	1.00
L64HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN62	HA	1.00	0.318	0.00	0.00
GLN62	HB2	0.72	0.026	1.00	0.94
GLN62	H	0.94	0.026	1.00	-827116.00
LEU63	HA	1.00	0.195	0.00	0.00
LEU63	HB2	1.00	0.004	1.00	0.43
LEU63	HB3	1.00	0.007	1.00	0.50
LEU63	HG	1.00	0.009	1.00	0.23
LEU63	HD11	0.99	0.006	1.00	0.35
LEU63	HD21	0.99	0.204	0.01	0.00
LEU63	H	1.00	0.013	1.00	-770813.00
LEU64	HA	1.00	0.155	0.00	0.00
LEU64	H	1.00	0.006	1.00	-318634.00

3.63.8 Detailed Probabilities of LEU63HB2:

Overall probability: 0.656

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU63	0.57	1.00
LEU64	0.95	1.00

Expected NOESY Contacts

Proton	Expected probability
L63HA	1.00
L63HB3	1.00
L63HG	1.00
L63HD11	1.00
L63HD21	1.00
L63H	1.00
L63HB2	1.00
L64H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU63	HA	1.00	0.220	0.00	0.00
LEU63	HB2	1.00	0.245	0.00	0.00
LEU63	HB3	1.00	0.001	1.00	1.81
LEU63	HG	1.00	0.023	1.00	1.00
LEU63	HD11	1.00	0.017	1.00	2.66
LEU63	HD21	1.00	0.258	0.00	0.00
LEU63	H	1.00	0.003	1.00	-722484.00
LEU64	H	1.00	0.031	0.90	0.00
LEU64	HA	0.65	0.025	1.00	0.87

3.63.9 Detailed Probabilities of LEU63HB3:

Overall probability: 0.863

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU63	0.84	1.00
LEU64	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L63HA	1.00
L63HB2	1.00
L63HG	1.00
L63HD11	1.00
L63HD21	1.00
L63H	1.00
L63HB3	1.00
L64H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU63	HA	1.00	0.006	1.00	0.79
LEU63	HB2	1.00	0.002	1.00	1.75
LEU63	HB3	1.00	0.031	0.90	0.00
LEU63	HG	1.00	0.002	1.00	0.91
LEU63	HD11	1.00	0.015	1.00	3.93
LEU63	HD21	1.00	0.244	0.00	0.00
LEU63	H	1.00	0.004	1.00	-549172.00
LEU64	H	1.00	0.007	1.00	-702735.00

3.63.10 Detailed Probabilities of LEU63HG:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU63	0.71	1.00
LEU64	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L63HA	1.00
L63HB2	1.00
L63HB3	1.00
L63HD11	1.00
L63HD21	1.00
L63H	1.00
L63HG	1.00
L64H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU63	HA	1.00	0.008	1.00	0.41
LEU63	HB2	1.00	0.006	1.00	0.78
LEU63	HB3	1.00	0.012	1.00	1.02
LEU63	HG	1.00	0.016	1.00	19.97
LEU63	HD11	1.00	0.108	0.00	0.00
LEU63	HD21	1.00	0.438	0.00	0.00
LEU63	H	1.00	0.007	1.00	-975670.00
LEU64	H	0.98	0.021	1.00	-1734049.00

3.63.11 Detailed Probabilities of LEU63HD11:

Overall probability: 0.572

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU63	0.57	1.00

Expected NOESY Contacts

Proton	Expected probability
L63HA	0.99
L63HB2	1.00
L63HB3	1.00
L63HG	1.00
L63HD12	1.00
L63HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU63	HA	0.99	0.691	0.01	0.00
LEU63	HB2	1.00	0.687	0.00	0.00
LEU63	HB3	1.00	0.015	1.00	1.16
LEU63	HG	1.00	0.006	1.00	1.18
LEU63	HD11	1.00	0.014	1.00	164.25
LEU63	HD21	1.00	0.129	0.00	0.00
LEU63	H	0.86	0.014	1.00	-554866.00

3.63.12 Detailed Probabilities of LEU63HD21:

Overall probability: 0.573

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU63	0.57	1.00

Expected NOESY Contacts

Proton	Expected probability
L63HA	0.99
L63HB2	1.00
L63HB3	1.00
L63HG	1.00
L63HD11	1.00
L63HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU63	HA	0.99	0.723	0.01	0.00
LEU63	HB2	1.00	0.719	0.00	0.00
LEU63	HB3	1.00	0.017	1.00	1.16
LEU63	HG	1.00	0.026	1.00	1.18
LEU63	HD11	1.00	0.018	1.00	164.25
LEU63	HD21	1.00	0.161	0.00	0.00
LEU63	H	0.85	0.018	1.00	-554866.00

3.63.13 Detailed Probabilities of LEU63H:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN62	1.00	1.00
LEU63	0.83	1.00
LEU64	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
Q62HG3	0.97
Q62HB3	1.00
Q62HA	1.00
Q62H	1.00
Q62HG2	0.98
L63HA	1.00
L63HB2	1.00
L63HB3	1.00
L63HG	1.00
L63H	1.00
L64H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN62	HA	1.00	0.000	1.00	0.52
GLN62	HB2	1.00	0.003	1.00	0.33
GLN62	HG2	0.98	0.006	1.00	0.08
GLN62	HG3	0.97	0.006	1.00	0.08
GLN62	H	1.00	0.001	1.00	-1691796.00
LEU63	HA	1.00	0.003	1.00	0.63
LEU63	HB2	1.00	0.005	1.00	0.67
LEU63	HB3	1.00	0.029	1.00	0.66
LEU63	HG	1.00	0.555	0.00	0.00
LEU63	H	1.00	0.001	1.00	-6075660.00
LEU63	HD21	0.87	0.024	1.00	0.42
LEU64	H	1.00	0.046	0.00	0.00
LEU64	HA	0.93	0.030	1.00	0.00
LEU64	HB2	0.64	0.029	1.00	0.53

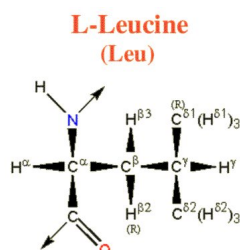
3.64 LEU(64)

Figure 63: Image from the BMRB

Residue probability: 0.789

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	172.526	177.056	1.929	0.000	0.000
CA 3.64.1	57.778	55.735	3.802	0.584	1.000
CB 3.64.2	41.350	42.389	3.750	0.778	1.000
CG 3.64.3	26.770	26.892	3.086	0.875	1.000
CD1 3.64.4	24.933	24.837	3.657	0.857	1.000
CD2 3.64.5	24.573	24.201	3.117	0.857	1.000
N 3.64.6	117.705	121.785	4.943	0.825	1.000
HA 3.64.7	3.907	4.315	0.840	0.709	1.000
HB2 3.64.8	1.789	1.601	0.373	0.625	1.000
HB3 3.64.9	1.629	1.508	0.398	0.875	1.000
HG 3.64.10	1.642	1.510	0.340	0.875	1.000
HD1 3.64.11	0.814	0.739	0.294	0.858	1.000
HD2 3.64.12	0.783	0.727	0.421	0.835	1.000
H 3.64.13	7.626	8.237	0.647	0.707	1.000

3.64.1 Detailed Probabilities of LEU64CA:

Overall probability: 0.584

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU63	0.67	1.00
LEU64	0.57	1.00
LYS65	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
L63HA	1.00
L64HB2	1.00
L64HB3	1.00
L64HG	1.00
L64HD11	0.99
L64HD21	0.99
L64H	1.00
L64HA	1.00
K65HA	1.00
K65H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU63	HA	1.00	0.155	0.00	0.00
LEU63	HB2	0.65	0.025	1.00	0.87
LEU63	H	0.93	0.030	1.00	0.00
LEU64	HA	1.00	0.382	0.00	0.00
LEU64	HB2	1.00	0.008	1.00	0.50
LEU64	HB3	1.00	0.008	1.00	0.71
LEU64	HG	1.00	0.005	1.00	0.71
LEU64	HD11	0.99	0.302	0.01	0.00
LEU64	HD21	0.99	0.271	0.01	0.00
LEU64	H	1.00	0.015	1.00	0.43
LYS65	HA	1.00	0.495	0.00	0.00
LYS65	H	1.00	0.027	1.00	0.28

3.64.2 Detailed Probabilities of LEU64CB:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU64	0.71	1.00
LYS65	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L64HA	1.00
L64HB2	1.00
L64HG	1.00
L64HD11	1.00
L64HD21	1.00
L64H	1.00
L64HB3	1.00
K65H	1.00

NOESY contacts detailed probability

3.64 LEU(64)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU64	HA	1.00	0.007	1.00	0.32
LEU64	HB2	1.00	0.001	1.00	1.28
LEU64	HB3	1.00	0.161	0.00	0.00
LEU64	HG	1.00	0.148	0.00	0.00
LEU64	HD11	1.00	0.011	1.00	0.91
LEU64	HD21	1.00	0.020	1.00	0.91
LEU64	H	1.00	0.018	1.00	0.42
LYS65	H	1.00	0.009	1.00	0.21
LYS65	HA	0.90	0.023	1.00	0.06

3.64.3 Detailed Probabilities of LEU64CG:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU64	0.86	1.00
LYS65	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L64HA	1.00
L64HB2	1.00
L64HB3	1.00
L64HD11	1.00
L64HD21	1.00
L64H	1.00
L64HG	1.00
K65H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU64	HA	1.00	0.008	1.00	0.27
LEU64	HB2	1.00	0.024	1.00	2.53
LEU64	HB3	1.00	0.007	1.00	19.97
LEU64	HG	1.00	0.006	1.00	19.97
LEU64	HD11	1.00	0.018	1.00	2.48
LEU64	HD21	1.00	0.013	1.00	2.48
LEU64	H	1.00	0.243	0.00	0.00
LYS65	H	0.98	0.017	1.00	0.53

3.64.4 Detailed Probabilities of LEU64CD1:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU64	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
L64HA	0.99
L64HB2	1.00
L64HB3	1.00
L64HG	1.00
L64HD12	1.00
L64HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU64	HA	0.99	0.010	1.00	0.89
LEU64	HB2	1.00	0.047	0.00	0.00
LEU64	HB3	1.00	0.014	1.00	4.39
LEU64	HG	1.00	0.001	1.00	4.39
LEU64	HD11	1.00	0.020	1.00	196.23
LEU64	HD21	1.00	0.011	1.00	196.23
LEU64	H	0.86	0.005	1.00	0.35

3.64.5 Detailed Probabilities of LEU64CD2:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU64	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
L64HA	0.99
L64HB2	1.00
L64HB3	1.00
L64HG	1.00
L64HD11	1.00
L64HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU64	HA	0.99	0.010	1.00	0.89
LEU64	HB2	1.00	0.465	0.00	0.00
LEU64	HB3	1.00	0.014	1.00	4.39
LEU64	HG	1.00	0.001	1.00	4.39
LEU64	HD11	1.00	0.020	1.00	196.23
LEU64	HD21	1.00	0.011	1.00	196.23
LEU64	H	0.85	0.005	1.00	0.35

3.64.6 Detailed Probabilities of LEU64N:

Overall probability: 0.825

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU63	0.78	1.00
LEU64	0.83	1.00
LYS65	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L63HB3	1.00
L63HB2	1.00
L63HA	1.00
L63H	1.00
L63HG	0.98
L64HA	1.00
L64HB2	1.00
L64HB3	1.00
L64HG	1.00
L64H	1.00
K65H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU63	HA	1.00	0.006	1.00	-318634.00
LEU63	HB2	1.00	0.031	0.90	0.00
LEU63	HB3	1.00	0.007	1.00	-702735.00
LEU63	HG	0.98	0.021	1.00	-1734049.00
LEU63	H	1.00	0.046	0.00	0.00
LEU64	HA	1.00	0.070	0.00	0.00
LEU64	HB2	1.00	0.005	1.00	-770738.00
LEU64	HB3	1.00	0.012	1.00	-1734049.00
LEU64	HG	1.00	0.001	1.00	-1734049.00
LEU64	H	1.00	0.016	1.00	-17911656.00
LEU64	HD11	0.88	0.016	1.00	-1748549.00
LYS65	H	1.00	0.008	1.00	-558677.00

3.64.7 Detailed Probabilities of LEU64HA:

Overall probability: 0.709

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU63	0.90	1.00
LEU64	0.71	1.00
LYS65	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
L63HA	1.00
L64HB2	1.00
L64HB3	1.00
L64HG	1.00
L64HD11	0.99
L64HD21	0.99
L64H	1.00
L64HA	1.00
K65HA	1.00
K65H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU63	HA	1.00	0.032	0.80	0.00
LEU63	HB2	0.65	0.010	1.00	0.05
LEU64	HA	1.00	0.382	0.00	0.00
LEU64	HB2	1.00	0.002	1.00	0.37
LEU64	HB3	1.00	0.007	1.00	0.32
LEU64	HG	1.00	0.008	1.00	0.27
LEU64	HD11	0.99	0.010	1.00	0.89
LEU64	HD21	0.99	0.010	1.00	0.89
LEU64	H	1.00	0.070	0.00	0.00
LYS65	HA	1.00	0.107	0.00	0.00
LYS65	H	1.00	0.006	1.00	-628522.00

3.64.8 Detailed Probabilities of LEU64HB2:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU64	0.57	1.00
LYS65	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L64HA	1.00
L64HB3	1.00
L64HG	1.00
L64HD11	1.00
L64HD21	1.00
L64H	1.00
L64HB2	1.00
K65H	1.00

NOESY contacts detailed probability

3.64 LEU(64)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU64	HA	1.00	0.008	1.00	0.50
LEU64	HB2	1.00	0.154	0.00	0.00
LEU64	HB3	1.00	0.001	1.00	1.28
LEU64	HG	1.00	0.024	1.00	2.53
LEU64	HD11	1.00	0.047	0.00	0.00
LEU64	HD21	1.00	0.465	0.00	0.00
LEU64	H	1.00	0.005	1.00	-770738.00
LYS65	H	1.00	0.020	1.00	-918305.00

3.64.9 Detailed Probabilities of LEU64HB3:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU64	0.86	1.00
LYS65	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L64HA	1.00
L64HB2	1.00
L64HG	1.00
L64HD11	1.00
L64HD21	1.00
L64H	1.00
L64HB3	1.00
K65H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU64	HA	1.00	0.008	1.00	0.71
LEU64	HB2	1.00	0.006	1.00	1.94
LEU64	HB3	1.00	0.161	0.00	0.00
LEU64	HG	1.00	0.007	1.00	19.97
LEU64	HD11	1.00	0.014	1.00	4.39
LEU64	HD21	1.00	0.014	1.00	4.39
LEU64	H	1.00	0.012	1.00	-1734049.00
LYS65	H	1.00	0.009	1.00	-843987.00

3.64.10 Detailed Probabilities of LEU64HG:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU64	0.86	1.00
LYS65	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L64HA	1.00
L64HB2	1.00
L64HB3	1.00
L64HD11	1.00
L64HD21	1.00
L64H	1.00
L64HG	1.00
K65H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU64	HA	1.00	0.005	1.00	0.71
LEU64	HB2	1.00	0.007	1.00	1.94
LEU64	HB3	1.00	0.148	0.00	0.00
LEU64	HG	1.00	0.006	1.00	19.97
LEU64	HD11	1.00	0.001	1.00	4.39
LEU64	HD21	1.00	0.001	1.00	4.39
LEU64	H	1.00	0.001	1.00	-1734049.00
LYS65	H	0.98	0.004	1.00	-843987.00

3.64.11 Detailed Probabilities of LEU64HD11:

Overall probability: 0.858

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU64	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
L64HA	0.99
L64HB2	1.00
L64HB3	1.00
L64HG	1.00
L64HD12	1.00
L64HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU64	HA	0.99	0.302	0.01	0.00
LEU64	HB2	1.00	0.010	1.00	1.00
LEU64	HB3	1.00	0.011	1.00	0.91
LEU64	HG	1.00	0.018	1.00	2.48
LEU64	HD11	1.00	0.020	1.00	196.23
LEU64	HD21	1.00	0.020	1.00	196.23
LEU64	H	0.86	0.016	1.00	-1748549.00

3.64.12 Detailed Probabilities of LEU64HD21:

Overall probability: 0.835

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU64	0.83	1.00

Expected NOESY Contacts

Proton	Expected probability
L64HA	0.99
L64HB2	1.00
L64HB3	1.00
L64HG	1.00
L64HD11	1.00
L64HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU64	HA	0.99	0.271	0.01	0.00
LEU64	HB2	1.00	0.021	1.00	1.00
LEU64	HB3	1.00	0.020	1.00	0.91
LEU64	HG	1.00	0.013	1.00	2.48
LEU64	HD11	1.00	0.011	1.00	196.23
LEU64	HD21	1.00	0.011	1.00	196.23

3.64.13 Detailed Probabilities of LEU64H:

Overall probability: 0.707

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU63	0.43	1.00
LEU64	0.86	1.00
LYS65	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L63HB3	1.00
L63HB2	1.00
L63HA	1.00
L63H	1.00
L63HG	0.98
L64HA	1.00
L64HB2	1.00
L64HB3	1.00
L64HG	1.00
L64H	1.00
K65H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU63	HA	1.00	0.042	0.00	0.00
LEU63	HB2	1.00	0.040	0.00	0.00
LEU63	HB3	1.00	0.016	1.00	0.66
LEU63	HG	0.98	0.510	0.02	0.00
LEU63	H	1.00	0.044	0.00	0.00
LEU63	HD11	0.53	0.007	1.00	0.45
LEU63	HD21	0.58	0.021	1.00	0.42
LEU64	HA	1.00	0.015	1.00	0.43
LEU64	HB2	1.00	0.016	1.00	0.53
LEU64	HB3	1.00	0.018	1.00	0.42
LEU64	HG	1.00	0.243	0.00	0.00
LEU64	H	1.00	0.016	1.00	-17911656.00
LEU64	HD11	0.88	0.005	1.00	0.35
LEU64	HD21	0.87	0.005	1.00	0.35
LYS65	H	1.00	0.016	1.00	-697715.00
LYS65	HA	0.89	0.018	1.00	0.97
LYS65	HB2	0.58	0.011	1.00	2.14

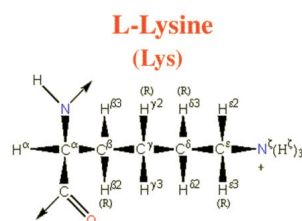


Figure 64: Image from the BMRB

Residue probability: 0.791
 Residue probability confidence: 0.943

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.479	176.660	3.133	0.000	0.000
CA 3.65.1	60.226	57.014	3.028	0.420	1.000
CB 3.65.2	32.266	32.981	3.186	0.840	1.000
CG 3.65.3	24.910	24.941	1.956	0.900	0.909
CD 3.65.4	29.497	29.020	2.193	0.744	0.889
CE 3.65.5	41.780	41.893	1.492	0.929	0.875
N 3.65.6	118.311	120.954	4.210	1.000	1.000
NZ	NA	—	—	0.000	0.000
HA 3.65.7	3.794	4.262	0.489	0.917	1.000
HB2 3.65.8	1.934	1.774	0.365	0.827	1.000
HB3 3.65.9	1.933	1.742	0.385	0.827	1.000
HG2 3.65.10	1.549	1.358	0.344	0.720	0.909
HG3 3.65.11	1.344	1.343	0.357	0.353	0.909
HD2 3.65.12	1.654	1.614	0.957	0.780	0.889
HD3 3.65.13	1.651	1.595	0.387	0.669	0.889
HE 3.65.14	2.916	2.907	0.230	1.000	0.875
H 3.65.15	8.038	8.185	0.605	0.938	1.000
HZ	NA	—	—	0.000	0.000

3.65.1 Detailed Probabilities of LYS65CA:

Overall probability: 0.420
 Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU64	0.50	1.00
LYS65	0.50	1.00
GLU66	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L64HA	1.00
K65HB2	1.00
K65HB3	1.00
K65HG2	1.00
K65HG3	1.00
K65HD2	0.98
K65HD3	0.98
K65H	1.00
K65HA	1.00
E66HA	1.00
E66H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU64	HA	1.00	0.107	0.00	0.00
LEU64	H	0.89	0.018	1.00	0.97
LYS65	HA	1.00	0.006	1.00	13.14
LYS65	HB2	1.00	0.376	0.00	0.00
LYS65	HB3	1.00	0.375	0.00	0.00
LYS65	HG2	1.00	0.009	1.00	0.96
LYS65	HG3	1.00	0.001	1.00	0.62
LYS65	HD2	0.98	0.096	0.02	0.00
LYS65	HD3	0.98	0.093	0.02	0.00
LYS65	H	1.00	0.007	1.00	0.77
GLU66	HA	1.00	0.085	0.00	0.00
GLU66	H	1.00	0.064	0.00	0.00

3.65.2 Detailed Probabilities of LYS65CB:

Overall probability: 0.840

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS65	0.82	1.00
GLU66	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K65HA	1.00
K65HB3	1.00
K65HG2	1.00
K65HG3	1.00
K65HD2	1.00
K65HD3	1.00
K65HE2	0.98
K65H	1.00
K65HB2	1.00
E66H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS65	HA	1.00	0.027	1.00	2.44
LYS65	HB2	1.00	0.030	1.00	0.00
LYS65	HB3	1.00	0.029	1.00	53.87
LYS65	HG2	1.00	0.034	0.60	0.00
LYS65	HG3	1.00	0.239	0.00	0.00
LYS65	HD2	1.00	0.029	1.00	5.56
LYS65	HD3	1.00	0.032	0.80	0.00
LYS65	HE2	0.99	0.013	1.00	0.70
LYS65	H	1.00	0.007	1.00	1.13
GLU66	H	1.00	0.004	1.00	2.95

3.65.3 Detailed Probabilities of LYS65CG:

Overall probability: 0.900

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS65	0.89	0.90
GLU66	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K65HA	1.00
K65HB2	1.00
K65HB3	1.00
K65HG2	1.00
K65HD2	1.00
K65HD3	1.00
K65HE2	1.00
K65H	1.00
K65HZ2	1.00
K65HG3	1.00
E66H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS65	HA	1.00	0.007	1.00	0.47
LYS65	HB2	1.00	0.004	1.00	2.40
LYS65	HB3	1.00	0.005	1.00	2.40
LYS65	HG2	1.00	0.017	1.00	4.89
LYS65	HG3	1.00	0.040	0.00	0.00
LYS65	HD2	1.00	0.019	1.00	9.44
LYS65	HD3	1.00	0.016	1.00	9.44
LYS65	HE2	1.00	0.002	1.00	0.63
LYS65	H	1.00	0.004	1.00	0.20
GLU66	H	0.97	0.011	1.00	0.36

3.65.4 Detailed Probabilities of LYS65CD:

Overall probability: 0.744

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS65	0.74	0.89

Expected NOESY Contacts

Proton	Expected probability
K65HA	0.98
K65HB2	1.00
K65HB3	1.00
K65HG2	1.00
K65HG3	1.00
K65HD3	1.00
K65HE2	1.00
K65HZ2	1.00
K65HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS65	HA	0.98	0.015	1.00	0.59
LYS65	HB2	1.00	0.002	1.00	5.45
LYS65	HB3	1.00	0.001	1.00	5.45
LYS65	HG2	1.00	0.146	0.00	0.00
LYS65	HG3	1.00	0.059	0.00	0.00
LYS65	HD2	1.00	0.030	1.00	0.00
LYS65	HD3	1.00	0.033	0.70	0.00
LYS65	HE2	1.00	0.003	1.00	4.26
LYS65	H	0.88	0.004	1.00	0.30

3.65.5 Detailed Probabilities of LYS65CE:

Overall probability: 0.929

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS65	0.93	0.88

Expected NOESY Contacts

Proton	Expected probability
K65HB2	0.98
K65HB3	0.99
K65HG2	1.00
K65HG3	1.00
K65HD2	1.00
K65HD3	1.00
K65HE3	1.00
K65HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS65	HB2	0.99	0.019	1.00	1.28
LYS65	HB3	0.99	0.018	1.00	1.28
LYS65	HG2	1.00	0.011	1.00	1.96
LYS65	HG3	1.00	0.035	0.50	0.00
LYS65	HD2	1.00	0.010	1.00	7.15
LYS65	HD3	1.00	0.013	1.00	7.15
LYS65	HE2	1.00	0.001	1.00	220.78

3.65.6 Detailed Probabilities of LYS65N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU64	1.00	1.00
LYS65	1.00	1.00
GLU66	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L64HA	1.00
L64H	1.00
L64HB3	1.00
L64HB2	1.00
L64HG	0.98
K65HA	1.00
K65HB2	1.00
K65HB3	1.00
K65HG2	1.00
K65HG3	1.00
K65H	1.00
E66H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU64	HA	1.00	0.006	1.00	-628522.00
LEU64	HB2	1.00	0.020	1.00	-918305.00
LEU64	HB3	1.00	0.009	1.00	-843987.00
LEU64	HG	0.98	0.004	1.00	-843987.00
LEU64	H	1.00	0.016	1.00	-697715.00
LYS65	HA	1.00	0.001	1.00	-895466.00
LYS65	HB2	1.00	0.008	1.00	-1375161.00
LYS65	HB3	1.00	0.009	1.00	-1375161.00
LYS65	HG2	1.00	0.009	1.00	-542976.00
LYS65	HG3	1.00	0.011	1.00	-263312.00
LYS65	H	1.00	0.005	1.00	-14033966.00
LYS65	HD2	0.88	0.016	1.00	-843987.00
LYS65	HD3	0.87	0.013	1.00	-843987.00
GLU66	H	1.00	0.009	1.00	-720051.00
GLU66	HB2	0.66	0.002	1.00	-914064.00

3.65.7 Detailed Probabilities of LYS65HA:

Overall probability: 0.917

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU64	0.50	1.00
LYS65	1.00	1.00
GLU66	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L64HA	1.00
K65HB2	1.00
K65HB3	1.00
K65HG2	1.00
K65HG3	1.00
K65HD2	0.98
K65HD3	0.98
K65H	1.00
K65HA	1.00
E66HA	1.00
E66H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU64	HA	1.00	0.495	0.00	0.00
LEU64	HB3	0.90	0.023	1.00	0.06
LYS65	HA	1.00	0.006	1.00	13.14
LYS65	HB2	1.00	0.027	1.00	2.44
LYS65	HB3	1.00	0.027	1.00	2.44
LYS65	HG2	1.00	0.003	1.00	0.84
LYS65	HG3	1.00	0.007	1.00	0.47
LYS65	HD2	0.98	0.015	1.00	0.59
LYS65	HD3	0.98	0.015	1.00	0.59
LYS65	H	1.00	0.001	1.00	-895466.00
GLU66	HA	1.00	0.019	1.00	0.18
GLU66	H	1.00	0.026	1.00	-359301.00

3.65.8 Detailed Probabilities of LYS65HB2:

Overall probability: 0.827

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS65	0.89	1.00
GLU66	0.55	1.00

Expected NOESY Contacts

Proton	Expected probability
K65HA	1.00
K65HB3	1.00
K65HG2	1.00
K65HG3	1.00
K65HD2	1.00
K65HD3	1.00
K65HE2	0.98
K65H	1.00
K65HB2	1.00
E66H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS65	HA	1.00	0.375	0.00	0.00
LYS65	HB2	1.00	0.029	1.00	53.87
LYS65	HB3	1.00	0.029	1.00	53.87
LYS65	HG2	1.00	0.015	1.00	2.64
LYS65	HG3	1.00	0.005	1.00	2.40
LYS65	HD2	1.00	0.001	1.00	5.45
LYS65	HD3	1.00	0.001	1.00	5.45
LYS65	HE2	0.99	0.018	1.00	1.28
LYS65	H	1.00	0.009	1.00	-1375161.00
GLU66	H	1.00	0.039	0.10	0.00
GLU66	HA	0.80	0.008	1.00	3.48

3.65.9 Detailed Probabilities of LYS65HB3:

Overall probability: 0.827

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS65	0.89	1.00
GLU66	0.55	1.00

Expected NOESY Contacts

Proton	Expected probability
K65HA	1.00
K65HB2	1.00
K65HG2	1.00
K65HG3	1.00
K65HD2	1.00
K65HD3	1.00
K65HE2	0.99
K65H	1.00
K65HB3	1.00
E66H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS65	HA	1.00	0.375	0.00	0.00
LYS65	HB2	1.00	0.029	1.00	53.87
LYS65	HB3	1.00	0.029	1.00	53.87
LYS65	HG2	1.00	0.015	1.00	2.64
LYS65	HG3	1.00	0.005	1.00	2.40
LYS65	HD2	1.00	0.001	1.00	5.45
LYS65	HD3	1.00	0.001	1.00	5.45
LYS65	HE2	0.99	0.018	1.00	1.28
LYS65	H	1.00	0.009	1.00	-1375161.00
GLU66	H	1.00	0.039	0.10	0.00
GLU66	HA	0.80	0.008	1.00	3.48

3.65.10 Detailed Probabilities of LYS65HG2:

Overall probability: 0.720

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS65	0.69	0.90
GLU66	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K65HA	1.00
K65HB2	1.00
K65HB3	1.00
K65HG3	1.00
K65HD2	1.00
K65HD3	1.00
K65HE2	1.00
K65H	1.00
K65HZ2	1.00
K65HG2	1.00
E66H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS65	HA	1.00	0.009	1.00	0.96
LYS65	HB2	1.00	0.034	0.60	0.00
LYS65	HB3	1.00	0.034	0.60	0.00
LYS65	HG2	1.00	0.011	1.00	37.64
LYS65	HG3	1.00	0.017	1.00	4.89
LYS65	HD2	1.00	0.146	0.00	0.00
LYS65	HD3	1.00	0.146	0.00	0.00
LYS65	HE2	1.00	0.011	1.00	1.96
LYS65	H	1.00	0.009	1.00	-542976.00
GLU66	H	0.98	0.018	1.00	-722584.00

3.65.11 Detailed Probabilities of LYS65HG3:

Overall probability: 0.353

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS65	0.39	0.90
GLU66	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
K65HA	1.00
K65HB2	1.00
K65HB3	1.00
K65HG2	1.00
K65HD2	1.00
K65HD3	1.00
K65HE2	1.00
K65H	1.00
K65HZ2	1.00
K65HG3	1.00
E66H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS65	HA	1.00	0.001	1.00	0.62
LYS65	HB2	1.00	0.239	0.00	0.00
LYS65	HB3	1.00	0.239	0.00	0.00
LYS65	HG2	1.00	0.028	1.00	5.85
LYS65	HG3	1.00	0.040	0.00	0.00
LYS65	HD2	1.00	0.059	0.00	0.00
LYS65	HD3	1.00	0.059	0.00	0.00
LYS65	HE2	1.00	0.035	0.50	0.00
LYS65	H	1.00	0.011	1.00	-263312.00
GLU66	H	0.97	0.051	0.03	0.00

3.65.12 Detailed Probabilities of LYS65HD2:

Overall probability: 0.780

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS65	0.78	0.89

Expected NOESY Contacts

Proton	Expected probability
K65HA	0.98
K65HB2	1.00
K65HB3	1.00
K65HG2	1.00
K65HG3	1.00
K65HD3	1.00
K65HE2	1.00
K65HZ2	1.00
K65HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS65	HA	0.98	0.096	0.02	0.00
LYS65	HB2	1.00	0.029	1.00	5.56
LYS65	HB3	1.00	0.029	1.00	5.56
LYS65	HG2	1.00	0.094	0.00	0.00
LYS65	HG3	1.00	0.019	1.00	9.44
LYS65	HD2	1.00	0.030	1.00	0.00
LYS65	HD3	1.00	0.030	1.00	0.00
LYS65	HE2	1.00	0.010	1.00	7.15
LYS65	H	0.88	0.016	1.00	-843987.00

3.65.13 Detailed Probabilities of LYS65HD3:

Overall probability: 0.669

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS65	0.67	0.89

Expected NOESY Contacts

Proton	Expected probability
K65HA	0.98
K65HB2	1.00
K65HB3	1.00
K65HG2	1.00
K65HG3	1.00
K65HD2	1.00
K65HE2	1.00
K65HZ2	1.00
K65HD3	1.00

NOESY contacts detailed probability

3.65 LYS(65)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS65	HA	0.98	0.093	0.02	0.00
LYS65	HB2	1.00	0.032	0.80	0.00
LYS65	HB3	1.00	0.032	0.80	0.00
LYS65	HG2	1.00	0.091	0.00	0.00
LYS65	HG3	1.00	0.016	1.00	9.44
LYS65	HD2	1.00	0.033	0.70	0.00
LYS65	HD3	1.00	0.033	0.70	0.00
LYS65	HE2	1.00	0.013	1.00	7.15
LYS65	H	0.87	0.013	1.00	-843987.00

3.65.14 Detailed Probabilities of LYS65HE2:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS65	1.00	0.88

Expected NOESY Contacts

Proton	Expected probability
K65HB2	0.98
K65HB3	0.99
K65HG2	1.00
K65HG3	1.00
K65HD2	1.00
K65HD3	1.00
K65HE3	1.00
K65HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS65	HB2	0.99	0.013	1.00	0.70
LYS65	HB3	0.99	0.013	1.00	0.70
LYS65	HG2	1.00	0.011	1.00	1.05
LYS65	HG3	1.00	0.002	1.00	0.63
LYS65	HD2	1.00	0.003	1.00	4.26
LYS65	HD3	1.00	0.003	1.00	4.26
LYS65	HE2	1.00	0.001	1.00	220.78

3.65.15 Detailed Probabilities of LYS65H:

Overall probability: 0.938

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU64	0.86	1.00
LYS65	1.00	1.00
GLU66	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L64HA	1.00
L64H	1.00
L64HB3	1.00
L64HB2	1.00
L64HG	0.98
K65HA	1.00
K65HB2	1.00
K65HB3	1.00
K65HG2	1.00
K65HG3	1.00
K65H	1.00
E66H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU64	HA	1.00	0.027	1.00	0.28
LEU64	HB2	1.00	0.396	0.00	0.00
LEU64	HB3	1.00	0.009	1.00	0.21
LEU64	HG	0.98	0.017	1.00	0.53
LEU64	H	1.00	0.008	1.00	-558677.00
LEU64	HD11	0.52	0.007	1.00	0.20
LEU64	HD21	0.59	0.007	1.00	0.20
LYS65	HA	1.00	0.007	1.00	0.77
LYS65	HB2	1.00	0.007	1.00	1.13
LYS65	HB3	1.00	0.007	1.00	1.13
LYS65	HG2	1.00	0.002	1.00	0.37
LYS65	HG3	1.00	0.004	1.00	0.20
LYS65	H	1.00	0.005	1.00	-14033966.00
LYS65	HD2	0.88	0.004	1.00	0.30
LYS65	HD3	0.87	0.004	1.00	0.30
GLU66	H	1.00	0.004	1.00	-750764.00

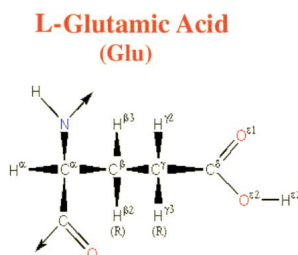


Figure 65: Image from the BMRB

Residue probability: 0.670
Residue probability confidence: 0.925

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.893	176.942	2.547	0.000	0.000
CA 3.66.1	59.119	57.442	3.837	0.809	1.000
CB 3.66.2	29.262	30.185	4.018	0.586	0.875
CG 3.66.3	36.010	36.085	1.533	0.857	0.875
N 3.66.4	119.362	120.574	4.837	0.542	1.000
HA 3.66.5	4.026	4.245	0.429	0.667	1.000
HB2 3.66.6	2.040	2.021	0.233	0.400	0.875
HB3 3.66.7	2.093	1.994	0.244	0.500	0.875
HG2 3.66.8	2.391	2.258	0.226	0.686	0.875
HG3 3.66.9	2.187	2.233	0.232	0.714	0.875
H 3.66.10	7.803	8.332	0.601	0.938	1.000
HE2	NA	—	—	0.000	0.000

3.66.1 Detailed Probabilities of GLU66CA:

Overall probability: 0.809
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS65	1.00	1.00
GLU66	0.82	1.00
MET67	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K65HA	1.00
E66HB2	1.00
E66HB3	1.00
E66HG2	1.00
E66HG3	1.00
E66H	1.00
E66HA	1.00
M67HA	1.00
M67H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS65	HA	1.00	0.019	1.00	0.18
LYS65	HB2	0.65	0.007	1.00	3.48
LYS65	HB3	0.80	0.008	1.00	3.48
GLU66	HA	1.00	0.016	1.00	41.95
GLU66	HB2	1.00	0.038	0.20	0.00
GLU66	HB3	1.00	0.015	1.00	5.05
GLU66	HG2	1.00	0.033	0.70	0.00
GLU66	HG3	1.00	0.022	1.00	2.61
GLU66	H	1.00	0.001	1.00	1.30
MET67	HA	1.00	0.094	0.00	0.00
MET67	H	1.00	0.006	1.00	0.35

3.66.2 Detailed Probabilities of GLU66CB:

Overall probability: 0.586

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU66	0.52	0.86
MET67	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E66HA	1.00
E66HB2	1.00
E66HG2	1.00
E66HG3	1.00
E66H	1.00
E66HE2	1.00
E66HB3	1.00
M67H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU66	HA	1.00	0.010	1.00	2.70
GLU66	HB2	1.00	0.053	0.00	0.00
GLU66	HB3	1.00	0.000	1.00	35.26
GLU66	HG2	1.00	0.039	0.10	0.00
GLU66	HG3	1.00	0.093	0.00	0.00
GLU66	H	1.00	0.007	1.00	0.96
MET67	H	1.00	0.006	1.00	0.45

3.66.3 Detailed Probabilities of GLU66CG:

Overall probability: 0.857

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU66	0.83	0.86
MET67	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E66HA	1.00
E66HB2	1.00
E66HB3	1.00
E66HG3	1.00
E66H	1.00
E66HE2	1.00
E66HG2	1.00
M67H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU66	HA	1.00	0.010	1.00	1.15
GLU66	HB2	1.00	0.095	0.00	0.00
GLU66	HB3	1.00	0.002	1.00	3.11
GLU66	HG2	1.00	0.000	1.00	30.23
GLU66	HG3	1.00	0.002	1.00	5.21
GLU66	H	1.00	0.016	1.00	0.49
MET67	H	0.98	0.008	1.00	0.13

3.66.4 Detailed Probabilities of GLU66N:

Overall probability: 0.542

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS65	0.64	1.00
GLU66	0.33	1.00
MET67	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K65HG3	0.97
K65HB2	1.00
K65HA	1.00
K65H	1.00
K65HB3	1.00
K65HG2	0.98
E66HA	1.00
E66HB2	1.00
E66HB3	1.00
E66HG2	1.00
E66HG3	1.00
E66H	1.00
M67H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS65	HA	1.00	0.026	1.00	-359301.00
LYS65	HB2	1.00	0.039	0.10	0.00
LYS65	HB3	1.00	0.040	0.00	0.00
LYS65	HG2	0.98	0.018	1.00	-722584.00
LYS65	HG3	0.97	0.051	0.03	0.00
LYS65	H	1.00	0.004	1.00	-750764.00
LYS65	HD2	0.59	0.018	1.00	-959776.00
LYS65	HD3	0.62	0.015	1.00	-959776.00
GLU66	HA	1.00	0.046	0.00	0.00
GLU66	HB2	1.00	0.067	0.00	0.00
GLU66	HB3	1.00	0.120	0.00	0.00
GLU66	HG2	1.00	0.005	1.00	-643869.00
GLU66	HG3	1.00	0.214	0.00	0.00
GLU66	H	1.00	0.006	1.00	-17394328.00
MET67	H	1.00	0.005	1.00	-847080.00

3.66.5 Detailed Probabilities of GLU66HA:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS65	0.00	1.00
GLU66	0.83	1.00
MET67	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K65HA	1.00
E66HB2	1.00
E66HB3	1.00
E66HG2	1.00
E66HG3	1.00
E66H	1.00
E66HA	1.00
M67HA	1.00
M67H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS65	HA	1.00	0.085	0.00	0.00
GLU66	HA	1.00	0.016	1.00	41.95
GLU66	HB2	1.00	0.010	1.00	2.70
GLU66	HB3	1.00	0.010	1.00	2.70
GLU66	HG2	1.00	0.010	1.00	1.15
GLU66	HG3	1.00	0.029	1.00	0.74
GLU66	H	1.00	0.046	0.00	0.00
MET67	HA	1.00	0.760	0.00	0.00
MET67	H	1.00	0.025	1.00	-269246.00

3.66.6 Detailed Probabilities of GLU66HB2:

Overall probability: 0.400

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU66	0.20	0.86
MET67	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E66HA	1.00
E66HB3	1.00
E66HG2	1.00
E66HG3	1.00
E66H	1.00
E66HE2	1.00
E66HB2	1.00
M67H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU66	HA	1.00	0.038	0.20	0.00
GLU66	HB2	1.00	0.001	1.00	52.03
GLU66	HB3	1.00	0.053	0.00	0.00
GLU66	HG2	1.00	0.095	0.00	0.00
GLU66	HG3	1.00	0.139	0.00	0.00
GLU66	H	1.00	0.067	0.00	0.00
MET67	H	1.00	0.009	1.00	-1416144.00
MET67	HA	0.69	0.030	1.00	0.44

3.66.7 Detailed Probabilities of GLU66HB3:

Overall probability: 0.500

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU66	0.50	0.86
MET67	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E66HA	1.00
E66HB2	1.00
E66HG2	1.00
E66HG3	1.00
E66H	1.00
E66HE2	1.00
E66HB3	1.00
M67H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU66	HA	1.00	0.015	1.00	5.05
GLU66	HB2	1.00	0.242	0.00	0.00
GLU66	HB3	1.00	0.000	1.00	35.26
GLU66	HG2	1.00	0.002	1.00	3.11
GLU66	HG3	1.00	0.100	0.00	0.00
GLU66	H	1.00	0.120	0.00	0.00
MET67	H	1.00	0.044	0.00	0.00
MET67	HA	0.86	0.023	1.00	0.44

3.66.8 Detailed Probabilities of GLU66HG2:

Overall probability: 0.686

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU66	0.63	0.86
MET67	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E66HA	1.00
E66HB2	1.00
E66HB3	1.00
E66HG3	1.00
E66H	1.00
E66HE2	1.00
E66HG2	1.00
M67H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU66	HA	1.00	0.033	0.70	0.00
GLU66	HB2	1.00	0.056	0.00	0.00
GLU66	HB3	1.00	0.039	0.10	0.00
GLU66	HG2	1.00	0.000	1.00	30.23
GLU66	HG3	1.00	0.002	1.00	5.81
GLU66	H	1.00	0.005	1.00	-643869.00
MET67	H	0.98	0.004	1.00	-441267.00

3.66.9 Detailed Probabilities of GLU66HG3:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU66	0.67	0.86
MET67	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E66HA	1.00
E66HB2	1.00
E66HB3	1.00
E66HG2	1.00
E66H	1.00
E66HE2	1.00
E66HG3	1.00
M67H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU66	HA	1.00	0.022	1.00	2.61
GLU66	HB2	1.00	0.005	1.00	14.03
GLU66	HB3	1.00	0.093	0.00	0.00
GLU66	HG2	1.00	0.002	1.00	5.21
GLU66	HG3	1.00	0.006	1.00	21.87
GLU66	H	1.00	0.214	0.00	0.00
MET67	H	0.97	0.014	1.00	-1155052.00

3.66.10 Detailed Probabilities of GLU66H:

Overall probability: 0.938

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS65	0.88	1.00
GLU66	1.00	1.00
MET67	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K65HG3	0.97
K65HB2	1.00
K65HA	1.00
K65H	1.00
K65HB3	1.00
K65HG2	0.98
E66HA	1.00
E66HB2	1.00
E66HB3	1.00
E66HG2	1.00
E66HG3	1.00
E66H	1.00
M67H	1.00

NOESY contacts detailed probability

3.66 GLU(66)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS65	HA	1.00	0.064	0.00	0.00
LYS65	HB2	1.00	0.004	1.00	2.95
LYS65	HB3	1.00	0.004	1.00	2.95
LYS65	HG2	0.98	0.001	1.00	0.50
LYS65	HG3	0.97	0.011	1.00	0.36
LYS65	H	1.00	0.009	1.00	-720051.00
LYS65	HD2	0.59	0.006	1.00	0.52
LYS65	HD3	0.62	0.006	1.00	0.52
GLU66	HA	1.00	0.001	1.00	1.30
GLU66	HB2	1.00	0.005	1.00	0.96
GLU66	HB3	1.00	0.007	1.00	0.96
GLU66	HG2	1.00	0.016	1.00	0.49
GLU66	HG3	1.00	0.011	1.00	0.40
GLU66	H	1.00	0.006	1.00	-17394328.00
MET67	H	1.00	0.007	1.00	-1019731.00
MET67	HA	0.91	0.026	1.00	0.09

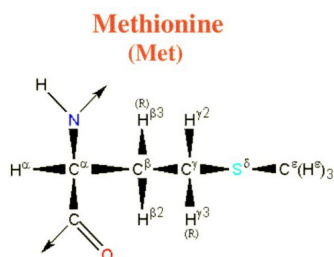


Figure 66: Image from the BMRB

Residue probability: 0.753
 Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	177.527	176.360	2.004	0.000	0.000
CA 3.67.1	59.963	56.303	4.222	0.750	1.000
CB 3.67.2	33.443	33.217	4.564	0.889	1.000
CG 3.67.3	32.070	32.123	4.122	0.877	1.000
CE 3.67.4	16.759	17.286	5.508	0.015	1.000
N 3.67.5	118.398	120.023	5.158	0.867	1.000
HA 3.67.6	3.948	4.409	0.504	0.778	1.000
HB2 3.67.7	2.203	2.016	0.340	0.893	1.000
HB3 3.67.8	2.049	1.978	0.359	0.892	1.000
HG2 3.67.9	2.567	2.410	0.360	0.752	1.000
HG3 3.67.10	2.395	2.378	0.386	0.875	1.000
HE 3.67.11	1.880	1.877	0.381	0.600	1.000
H 3.67.12	8.394	8.269	0.585	0.846	1.000

3.67.1 Detailed Probabilities of MET67CA:

Overall probability: 0.750
 Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU66	0.75	1.00
MET67	0.83	1.00
LEU68	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E66HA	1.00
M67HB2	1.00
M67HB3	1.00
M67HG2	1.00
M67HG3	1.00
M67H	1.00
M67HA	1.00
L68HA	1.00
L68H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU66	HA	1.00	0.760	0.00	0.00
GLU66	HB2	0.69	0.030	1.00	0.44
GLU66	HB3	0.86	0.023	1.00	0.44
GLU66	H	0.91	0.026	1.00	0.09
MET67	HA	1.00	0.838	0.00	0.00
MET67	HB2	1.00	0.018	1.00	0.72
MET67	HB3	1.00	0.021	1.00	0.44
MET67	HG2	1.00	0.024	1.00	0.38
MET67	HG3	1.00	0.003	1.00	0.47
MET67	H	1.00	0.013	1.00	0.53
LEU68	HA	1.00	1.007	0.00	0.00
LEU68	H	1.00	0.011	1.00	0.16

3.67.2 Detailed Probabilities of MET67CB:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET67	1.00	1.00
LEU68	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
M67HA	1.00
M67HB2	1.00
M67HG2	1.00
M67HG3	1.00
M67HE1	0.97
M67H	1.00
M67HB3	1.00
L68H	1.00

NOESY contacts detailed probability

3.67 MET(67)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET67	HA	1.00	0.004	1.00	0.55
MET67	HB2	1.00	0.001	1.00	4.01
MET67	HB3	1.00	0.013	1.00	7.54
MET67	HG2	1.00	0.022	1.00	0.12
MET67	HG3	1.00	0.013	1.00	1.05
MET67	HE1	0.97	0.026	1.00	0.32
MET67	H	1.00	0.012	1.00	0.30
LEU68	H	1.00	0.065	0.00	0.00
LEU68	HA	0.84	0.015	1.00	0.06

3.67.3 Detailed Probabilities of MET67CG:

Overall probability: 0.877

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET67	1.00	1.00
LEU68	0.01	1.00

Expected NOESY Contacts

Proton	Expected probability
M67HA	1.00
M67HB2	1.00
M67HB3	1.00
M67HG3	1.00
M67HE1	1.00
M67H	1.00
M67HG2	1.00
L68H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET67	HA	1.00	0.006	1.00	0.39
MET67	HB2	1.00	0.002	1.00	0.54
MET67	HB3	1.00	0.001	1.00	0.24
MET67	HG2	1.00	0.001	1.00	5.98
MET67	HG3	1.00	0.003	1.00	2.69
MET67	HE1	1.00	0.002	1.00	0.55
MET67	H	1.00	0.005	1.00	0.27
LEU68	H	0.99	0.072	0.01	0.00

3.67.4 Detailed Probabilities of MET67CE:

Overall probability: 0.015

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET67	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
M67HB2	0.96
M67HB3	0.97
M67HG2	1.00
M67HG3	1.00
M67HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET67	HB2	0.96	0.409	0.04	0.00
MET67	HB3	0.97	0.255	0.03	0.00
MET67	HG2	1.00	0.373	0.00	0.00
MET67	HG3	1.00	0.545	0.00	0.00
MET67	HE1	1.00	0.086	0.00	0.00

3.67.5 Detailed Probabilities of MET67N:

Overall probability: 0.867

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU66	0.83	1.00
MET67	1.00	1.00
LEU68	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
E66HB2	1.00
E66HA	1.00
E66HG3	0.97
E66HB3	1.00
E66H	1.00
E66HG2	0.98
M67HA	1.00
M67HB2	1.00
M67HB3	1.00
M67HG2	1.00
M67HG3	1.00
M67H	1.00
L68H	1.00

NOESY contacts detailed probability

3.67 MET(67)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU66	HA	1.00	0.025	1.00	-269246.00
GLU66	HB2	1.00	0.009	1.00	-1416144.00
GLU66	HB3	1.00	0.044	0.00	0.00
GLU66	HG2	0.98	0.004	1.00	-441267.00
GLU66	HG3	0.97	0.014	1.00	-1155052.00
GLU66	H	1.00	0.007	1.00	-1019731.00
MET67	HA	1.00	0.000	1.00	-845525.00
MET67	HB2	1.00	0.002	1.00	-1155052.00
MET67	HB3	1.00	0.000	1.00	-1416144.00
MET67	HG2	1.00	0.000	1.00	-419223.00
MET67	HG3	1.00	0.000	1.00	-441267.00
MET67	H	1.00	0.005	1.00	-7152006.00
LEU68	H	1.00	0.065	0.00	0.00
LEU68	HA	0.93	0.006	1.00	-128672.00
LEU68	HB2	0.63	0.004	1.00	-82596.00

3.67.6 Detailed Probabilities of MET67HA:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU66	0.00	1.00
MET67	0.83	1.00
LEU68	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E66HA	1.00
M67HB2	1.00
M67HB3	1.00
M67HG2	1.00
M67HG3	1.00
M67H	1.00
M67HA	1.00
L68HA	1.00
L68H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU66	HA	1.00	0.094	0.00	0.00
MET67	HA	1.00	0.838	0.00	0.00
MET67	HB2	1.00	0.001	1.00	0.41
MET67	HB3	1.00	0.004	1.00	0.55
MET67	HG2	1.00	0.006	1.00	0.39
MET67	HG3	1.00	0.006	1.00	0.38
MET67	H	1.00	0.000	1.00	-845525.00
LEU68	HA	1.00	0.020	1.00	0.19
LEU68	H	1.00	0.002	1.00	-284714.00

3.67.7 Detailed Probabilities of MET67HB2:

Overall probability: 0.893

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET67	0.86	1.00
LEU68	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
M67HA	1.00
M67HB3	1.00
M67HG2	1.00
M67HG3	1.00
M67HE1	0.96
M67H	1.00
M67HB2	1.00
L68H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET67	HA	1.00	0.018	1.00	0.72
MET67	HB2	1.00	0.001	1.00	7.09
MET67	HB3	1.00	0.001	1.00	4.01
MET67	HG2	1.00	0.002	1.00	0.54
MET67	HG3	1.00	0.000	1.00	0.56
MET67	HE1	0.96	0.409	0.04	0.00
MET67	H	1.00	0.002	1.00	-1155052.00
LEU68	H	1.00	0.004	1.00	-485003.00
LEU68	HA	0.66	0.022	1.00	0.08

3.67.8 Detailed Probabilities of MET67HB3:

Overall probability: 0.892

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET67	0.86	1.00
LEU68	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
M67HA	1.00
M67HB2	1.00
M67HG2	1.00
M67HG3	1.00
M67HE1	0.97
M67H	1.00
M67HB3	1.00
L68H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET67	HA	1.00	0.021	1.00	0.44
MET67	HB2	1.00	0.011	1.00	4.04
MET67	HB3	1.00	0.013	1.00	7.54
MET67	HG2	1.00	0.001	1.00	0.24
MET67	HG3	1.00	0.001	1.00	0.32
MET67	HE1	0.97	0.255	0.03	0.00
MET67	H	1.00	0.000	1.00	-1416144.00
LEU68	H	1.00	0.000	1.00	-600234.00
LEU68	HA	0.84	0.002	1.00	0.11

3.67.9 Detailed Probabilities of MET67HG2:

Overall probability: 0.752

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET67	0.86	1.00
LEU68	0.01	1.00

Expected NOESY Contacts

Proton	Expected probability
M67HA	1.00
M67HB2	1.00
M67HB3	1.00
M67HG3	1.00
M67HE1	1.00
M67H	1.00
M67HG2	1.00
L68H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET67	HA	1.00	0.024	1.00	0.38
MET67	HB2	1.00	0.027	1.00	0.47
MET67	HB3	1.00	0.022	1.00	0.12
MET67	HG2	1.00	0.001	1.00	5.98
MET67	HG3	1.00	0.010	1.00	3.18
MET67	HE1	1.00	0.373	0.00	0.00
MET67	H	1.00	0.000	1.00	-419223.00
LEU68	H	0.99	0.167	0.01	0.00

3.67.10 Detailed Probabilities of MET67HG3:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET67	0.86	1.00
LEU68	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
M67HA	1.00
M67HB2	1.00
M67HB3	1.00
M67HG2	1.00
M67HE1	1.00
M67H	1.00
M67HG3	1.00
L68H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET67	HA	1.00	0.003	1.00	0.47
MET67	HB2	1.00	0.014	1.00	1.43
MET67	HB3	1.00	0.013	1.00	1.05
MET67	HG2	1.00	0.003	1.00	2.69
MET67	HG3	1.00	0.000	1.00	3.06
MET67	HE1	1.00	0.545	0.00	0.00
MET67	H	1.00	0.000	1.00	-441267.00
LEU68	H	0.98	0.005	1.00	-167519.00

3.67.11 Detailed Probabilities of MET67HE1:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET67	0.60	1.00

Expected NOESY Contacts

Proton	Expected probability
M67HB2	0.96
M67HB3	0.97
M67HG2	1.00
M67HG3	1.00
M67HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET67	HB2	0.96	0.007	1.00	0.32
MET67	HB3	0.97	0.026	1.00	0.32
MET67	HG2	1.00	0.002	1.00	0.55
MET67	HG3	1.00	0.152	0.00	0.00
MET67	HE1	1.00	0.086	0.00	0.00

3.67.12 Detailed Probabilities of MET67H:

Overall probability: 0.846

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU66	0.83	1.00
MET67	1.00	1.00
LEU68	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E66HB2	1.00
E66HA	1.00
E66HG3	0.97
E66HB3	1.00
E66H	1.00
E66HG2	0.98
M67HA	1.00
M67HB2	1.00
M67HB3	1.00
M67HG2	1.00
M67HG3	1.00
M67H	1.00
L68H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU66	HA	1.00	0.006	1.00	0.35
GLU66	HB2	1.00	0.298	0.00	0.00
GLU66	HB3	1.00	0.006	1.00	0.45
GLU66	HG2	0.98	0.008	1.00	0.13
GLU66	HG3	0.97	0.010	1.00	0.16
GLU66	H	1.00	0.005	1.00	-847080.00
MET67	HA	1.00	0.013	1.00	0.53
MET67	HB2	1.00	0.005	1.00	0.32
MET67	HB3	1.00	0.012	1.00	0.30
MET67	HG2	1.00	0.005	1.00	0.27
MET67	HG3	1.00	0.012	1.00	0.15
MET67	H	1.00	0.005	1.00	-7152006.00
LEU68	H	1.00	0.076	0.00	0.00

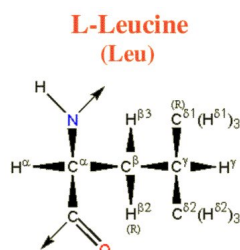
3.68 LEU(68)

Figure 67: Image from the BMRB

Residue probability: 0.835

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.869	177.056	1.929	0.000	0.000
CA 3.68.1	57.941	55.735	3.802	0.917	1.000
CB 3.68.2	40.875	42.389	3.750	0.875	1.000
CG 3.68.3	26.447	26.892	3.086	0.378	1.000
CD1 3.68.4	25.266	24.837	3.657	1.000	1.000
CD2 3.68.5	23.070	24.201	3.117	1.000	1.000
N 3.68.6	118.269	121.785	4.943	0.868	1.000
HA 3.68.7	3.779	4.315	0.840	0.883	1.000
HB2 3.68.8	1.747	1.601	0.373	0.875	1.000
HB3 3.68.9	1.381	1.508	0.398	0.889	1.000
HG 3.68.10	1.588	1.510	0.340	0.503	1.000
HD1 3.68.11	0.507	0.739	0.294	1.000	1.000
HD2 3.68.12	0.384	0.727	0.421	1.000	1.000
H 3.68.13	8.471	8.237	0.647	0.668	1.000

3.68.1 Detailed Probabilities of LEU68CA:

Overall probability: 0.917

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET67	1.00	1.00
LEU68	1.00	1.00
GLU69	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
M67HA	1.00
L68HB2	1.00
L68HB3	1.00
L68HG	1.00
L68HD11	0.99
L68HD21	0.99
L68H	1.00
L68HA	1.00
E69HA	1.00
E69H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET67	HA	1.00	0.020	1.00	0.19
MET67	HB2	0.66	0.022	1.00	0.08
MET67	HB3	0.84	0.002	1.00	0.11
LEU68	HA	1.00	0.001	1.00	3.73
LEU68	HB2	1.00	0.019	1.00	0.47
LEU68	HB3	1.00	0.003	1.00	0.48
LEU68	HG	1.00	0.008	1.00	0.34
LEU68	HD11	0.99	0.007	1.00	0.29
LEU68	HD21	0.99	0.003	1.00	1.09
LEU68	H	1.00	0.003	1.00	0.40
GLU69	HA	1.00	0.127	0.00	0.00
GLU69	H	1.00	0.015	1.00	0.14

3.68.2 Detailed Probabilities of LEU68CB:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU68	0.86	1.00
GLU69	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L68HA	1.00
L68HB2	1.00
L68HG	1.00
L68HD11	1.00
L68HD21	1.00
L68H	1.00
L68HB3	1.00
E69H	1.00

NOESY contacts detailed probability

3.68 LEU(68)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU68	HA	1.00	0.005	1.00	0.66
LEU68	HB2	1.00	0.008	1.00	3.76
LEU68	HB3	1.00	0.014	1.00	5.42
LEU68	HG	1.00	0.044	0.00	0.00
LEU68	HD11	1.00	0.005	1.00	0.61
LEU68	HD21	1.00	0.003	1.00	0.54
LEU68	H	1.00	0.001	1.00	0.42
GLU69	H	1.00	0.015	1.00	0.66

3.68.3 Detailed Probabilities of LEU68CG:

Overall probability: 0.378

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU68	0.43	1.00
GLU69	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
L68HA	1.00
L68HB2	1.00
L68HB3	1.00
L68HD11	1.00
L68HD21	1.00
L68H	1.00
L68HG	1.00
E69H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU68	HA	1.00	0.009	1.00	0.27
LEU68	HB2	1.00	0.101	0.00	0.00
LEU68	HB3	1.00	0.467	0.00	0.00
LEU68	HG	1.00	0.260	0.00	0.00
LEU68	HD11	1.00	0.005	1.00	0.40
LEU68	HD21	1.00	0.005	1.00	0.57
LEU68	H	1.00	0.070	0.00	0.00
GLU69	H	0.98	0.618	0.02	0.00

3.68.4 Detailed Probabilities of LEU68CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU68	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L68HA	0.99
L68HB2	1.00
L68HB3	1.00
L68HG	1.00
L68HD12	1.00
L68HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU68	HA	0.99	0.014	1.00	0.58
LEU68	HB2	1.00	0.004	1.00	0.58
LEU68	HB3	1.00	0.007	1.00	0.52
LEU68	HG	1.00	0.006	1.00	0.76
LEU68	HD11	1.00	0.005	1.00	26.19
LEU68	HD21	1.00	0.003	1.00	1.80
LEU68	H	0.86	0.002	1.00	0.15

3.68.5 Detailed Probabilities of LEU68CD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU68	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L68HA	0.99
L68HB2	1.00
L68HB3	1.00
L68HG	1.00
L68HD11	1.00
L68HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU68	HA	0.99	0.007	1.00	1.14
LEU68	HB2	1.00	0.003	1.00	0.39
LEU68	HB3	1.00	0.010	1.00	0.59
LEU68	HG	1.00	0.005	1.00	0.92
LEU68	HD11	1.00	0.009	1.00	1.80
LEU68	HD21	1.00	0.002	1.00	30.62
LEU68	H	0.85	0.007	1.00	0.21

3.68.6 Detailed Probabilities of LEU68N:

Overall probability: 0.868

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET67	0.67	1.00
LEU68	1.00	1.00
GLU69	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
M67HG2	0.99
M67HB2	1.00
M67HA	1.00
M67HB3	1.00
M67H	1.00
M67HG3	0.98
L68HA	1.00
L68HB2	1.00
L68HB3	1.00
L68HG	1.00
L68H	1.00
E69H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET67	HA	1.00	0.002	1.00	-284714.00
MET67	HB2	1.00	0.004	1.00	-485003.00
MET67	HB3	1.00	0.000	1.00	-600234.00
MET67	HG2	0.99	0.167	0.01	0.00
MET67	HG3	0.98	0.005	1.00	-167519.00
MET67	H	1.00	0.076	0.00	0.00
LEU68	HA	1.00	0.007	1.00	-832352.00
LEU68	HB2	1.00	0.004	1.00	-871434.00
LEU68	HB3	1.00	0.003	1.00	-612975.00
LEU68	HG	1.00	0.005	1.00	-986313.00
LEU68	H	1.00	0.001	1.00	-6357373.00
LEU68	HD11	0.88	0.003	1.00	-393886.00
LEU68	HD21	0.87	0.003	1.00	-336840.00
GLU69	H	1.00	0.007	1.00	-758646.00
GLU69	HB2	0.55	0.002	1.00	-485003.00

3.68.7 Detailed Probabilities of LEU68HA:

Overall probability: 0.883

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET67	0.67	1.00
LEU68	1.00	1.00
GLU69	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
M67HA	1.00
L68HB2	1.00
L68HB3	1.00
L68HG	1.00
L68HD11	0.99
L68HD21	0.99
L68H	1.00
L68HA	1.00
E69HA	1.00
E69H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET67	HA	1.00	1.007	0.00	0.00
MET67	HB3	0.84	0.015	1.00	0.06
MET67	H	0.93	0.006	1.00	-128672.00
LEU68	HA	1.00	0.001	1.00	3.73
LEU68	HB2	1.00	0.008	1.00	0.65
LEU68	HB3	1.00	0.005	1.00	0.66
LEU68	HG	1.00	0.009	1.00	0.27
LEU68	HD11	0.99	0.014	1.00	0.58
LEU68	HD21	0.99	0.007	1.00	1.14
LEU68	H	1.00	0.007	1.00	-832352.00
GLU69	HA	1.00	0.034	0.60	0.00
GLU69	H	1.00	0.019	1.00	-867318.00

3.68.8 Detailed Probabilities of LEU68HB2:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU68	0.86	1.00
GLU69	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L68HA	1.00
L68HB3	1.00
L68HG	1.00
L68HD11	1.00
L68HD21	1.00
L68H	1.00
L68HB2	1.00
E69H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU68	HA	1.00	0.019	1.00	0.47
LEU68	HB2	1.00	0.008	1.00	4.26
LEU68	HB3	1.00	0.008	1.00	3.76
LEU68	HG	1.00	0.101	0.00	0.00
LEU68	HD11	1.00	0.004	1.00	0.58
LEU68	HD21	1.00	0.003	1.00	0.39
LEU68	H	1.00	0.004	1.00	-871434.00
GLU69	H	1.00	0.001	1.00	-509652.00

3.68.9 Detailed Probabilities of LEU68HB3:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU68	0.86	1.00
GLU69	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L68HA	1.00
L68HB2	1.00
L68HG	1.00
L68HD11	1.00
L68HD21	1.00
L68H	1.00
L68HB3	1.00
E69H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU68	HA	1.00	0.003	1.00	0.48
LEU68	HB2	1.00	0.010	1.00	3.70
LEU68	HB3	1.00	0.014	1.00	5.42
LEU68	HG	1.00	0.467	0.00	0.00
LEU68	HD11	1.00	0.007	1.00	0.52
LEU68	HD21	1.00	0.010	1.00	0.59
LEU68	H	1.00	0.003	1.00	-612975.00
GLU69	H	1.00	0.002	1.00	-388179.00
GLU69	HA	0.90	0.023	1.00	1.34

3.68.10 Detailed Probabilities of LEU68HG:

Overall probability: 0.503

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU68	0.57	1.00
GLU69	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
L68HA	1.00
L68HB2	1.00
L68HB3	1.00
L68HD11	1.00
L68HD21	1.00
L68H	1.00
L68HG	1.00
E69H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU68	HA	1.00	0.008	1.00	0.34
LEU68	HB2	1.00	0.040	0.00	0.00
LEU68	HB3	1.00	0.044	0.00	0.00
LEU68	HG	1.00	0.260	0.00	0.00
LEU68	HD11	1.00	0.006	1.00	0.76
LEU68	HD21	1.00	0.005	1.00	0.92
LEU68	H	1.00	0.005	1.00	-986313.00
GLU69	H	0.98	0.040	0.02	0.00

3.68.11 Detailed Probabilities of LEU68HD11:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU68	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L68HA	0.99
L68HB2	1.00
L68HB3	1.00
L68HG	1.00
L68HD12	1.00
L68HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU68	HA	0.99	0.007	1.00	0.29
LEU68	HB2	1.00	0.005	1.00	0.70
LEU68	HB3	1.00	0.005	1.00	0.61
LEU68	HG	1.00	0.005	1.00	0.40
LEU68	HD11	1.00	0.005	1.00	26.19
LEU68	HD21	1.00	0.009	1.00	1.80
LEU68	H	0.86	0.003	1.00	-393886.00

3.68.12 Detailed Probabilities of LEU68HD21:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU68	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L68HA	0.99
L68HB2	1.00
L68HB3	1.00
L68HG	1.00
L68HD11	1.00
L68HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU68	HA	0.99	0.003	1.00	1.09
LEU68	HB2	1.00	0.003	1.00	0.50
LEU68	HB3	1.00	0.003	1.00	0.54
LEU68	HG	1.00	0.005	1.00	0.57
LEU68	HD11	1.00	0.003	1.00	1.80
LEU68	HD21	1.00	0.002	1.00	30.62
LEU68	H	0.85	0.003	1.00	-336840.00

3.68.13 Detailed Probabilities of LEU68H:

Overall probability: 0.668

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET67	0.34	1.00
LEU68	0.86	1.00
GLU69	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
M67HG2	0.99
M67HB2	1.00
M67HA	1.00
M67HB3	1.00
M67H	1.00
M67HG3	0.98
L68HA	1.00
L68HB2	1.00
L68HB3	1.00
L68HG	1.00
L68H	1.00
E69H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET67	HA	1.00	0.011	1.00	0.16
MET67	HB2	1.00	0.082	0.00	0.00
MET67	HB3	1.00	0.065	0.00	0.00
MET67	HG2	0.99	0.072	0.01	0.00
MET67	HG3	0.98	0.020	1.00	0.08
MET67	H	1.00	0.065	0.00	0.00
LEU68	HA	1.00	0.003	1.00	0.40
LEU68	HB2	1.00	0.002	1.00	0.55
LEU68	HB3	1.00	0.001	1.00	0.42
LEU68	HG	1.00	0.070	0.00	0.00
LEU68	H	1.00	0.001	1.00	-6357373.00
LEU68	HD11	0.88	0.002	1.00	0.15
LEU68	HD21	0.87	0.007	1.00	0.21
GLU69	H	1.00	0.000	1.00	-729112.00
GLU69	HB2	0.55	0.009	1.00	0.06

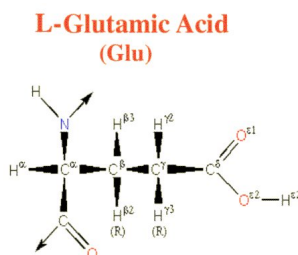
3.69 GLU(69)

Figure 68: Image from the BMRB

Residue probability: 0.780

Residue probability confidence: 0.925

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	179.063	176.942	2.547	0.000	0.000
CA 3.69.1	59.424	57.442	3.837	0.700	1.000
CB 3.69.2	29.140	30.185	4.018	0.838	0.875
CG 3.69.3	36.010	36.085	1.533	0.857	0.875
N 3.69.4	118.681	120.574	4.837	0.823	1.000
HA 3.69.5	4.055	4.245	0.429	0.778	1.000
HB2 3.69.6	2.201	2.021	0.233	0.486	0.875
HB3 3.69.7	2.089	1.994	0.244	0.900	0.875
HG2 3.69.8	2.273	2.258	0.226	0.574	0.875
HG3 3.69.9	2.437	2.233	0.232	1.000	0.875
H 3.69.10	7.627	8.332	0.601	0.848	1.000
HE2	NA	—	—	0.000	0.000

3.69.1 Detailed Probabilities of GLU69CA:

Overall probability: 0.700

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU68	0.80	1.00
GLU69	0.90	1.00
LEU70	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L68HA	1.00
E69HB2	1.00
E69HB3	1.00
E69HG2	1.00
E69HG3	1.00
E69H	1.00
E69HA	1.00
L70H	1.00
L70HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU68	HA	1.00	0.034	0.60	0.00
LEU68	HB3	0.90	0.023	1.00	1.34
GLU69	HA	1.00	0.013	1.00	41.95
GLU69	HB2	1.00	0.036	0.40	0.00
GLU69	HB3	1.00	0.011	1.00	5.05
GLU69	HG2	1.00	0.009	1.00	2.14
GLU69	HG3	1.00	0.013	1.00	1.54
GLU69	H	1.00	0.001	1.00	0.91
LEU70	HA	1.00	0.119	0.00	0.00
LEU70	H	1.00	0.085	0.00	0.00

3.69.2 Detailed Probabilities of GLU69CB:

Overall probability: 0.838

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU69	0.78	0.86
LEU70	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E69HA	1.00
E69HB3	1.00
E69HG2	1.00
E69HG3	1.00
E69H	1.00
E69HE2	1.00
E69HB2	1.00
L70H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU69	HA	1.00	0.008	1.00	1.52
GLU69	HB2	1.00	0.019	1.00	19.33
GLU69	HB3	1.00	0.033	0.70	0.00
GLU69	HG2	1.00	0.077	0.00	0.00
GLU69	HG3	1.00	0.024	1.00	2.85
GLU69	H	1.00	0.005	1.00	0.92
LEU70	H	1.00	0.011	1.00	0.38
LEU70	HA	0.68	0.027	1.00	0.58

3.69.3 Detailed Probabilities of GLU69CG:

Overall probability: 0.857

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU69	0.83	0.86
LEU70	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E69HA	1.00
E69HB2	1.00
E69HB3	1.00
E69HG2	1.00
E69H	1.00
E69HE2	1.00
E69HG3	1.00
L70H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU69	HA	1.00	0.010	1.00	1.15
GLU69	HB2	1.00	0.082	0.00	0.00
GLU69	HB3	1.00	0.002	1.00	3.11
GLU69	HG2	1.00	0.010	1.00	6.47
GLU69	HG3	1.00	0.008	1.00	35.10
GLU69	H	1.00	0.008	1.00	0.71
LEU70	H	0.97	0.014	1.00	0.17

3.69.4 Detailed Probabilities of GLU69N:

Overall probability: 0.823

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU68	0.86	1.00
GLU69	0.77	1.00
LEU70	0.90	1.00

Expected NOESY Contacts

Proton	Expected probability
L68HA	1.00
L68HB2	1.00
L68HB3	1.00
L68HG	0.98
L68H	1.00
E69HA	1.00
E69HB2	1.00
E69HB3	1.00
E69HG2	1.00
E69HG3	1.00
E69H	1.00
L70H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU68	HA	1.00	0.019	1.00	-867318.00
LEU68	HB2	1.00	0.001	1.00	-509652.00
LEU68	HB3	1.00	0.002	1.00	-388179.00
LEU68	HG	0.98	0.040	0.02	0.00
LEU68	H	1.00	0.000	1.00	-729112.00
LEU68	HD11	0.51	0.008	1.00	-145245.00
LEU68	HD21	0.58	0.004	1.00	-132745.00
GLU69	HA	1.00	0.012	1.00	-1383855.00
GLU69	HB2	1.00	0.000	1.00	-1353797.00
GLU69	HB3	1.00	0.034	0.60	0.00
GLU69	HG2	1.00	0.072	0.00	0.00
GLU69	HG3	1.00	0.001	1.00	-613247.00
GLU69	H	1.00	0.017	1.00	-19107776.00
LEU70	H	1.00	0.031	0.90	0.00

3.69.5 Detailed Probabilities of GLU69HA:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU68	0.00	1.00
GLU69	1.00	1.00
LEU70	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
L68HA	1.00
E69HB2	1.00
E69HB3	1.00
E69HG2	1.00
E69HG3	1.00
E69H	1.00
E69HA	1.00
L70H	1.00
L70HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU68	HA	1.00	0.127	0.00	0.00
GLU69	HA	1.00	0.013	1.00	41.95
GLU69	HB2	1.00	0.008	1.00	1.52
GLU69	HB3	1.00	0.019	1.00	2.70
GLU69	HG2	1.00	0.018	1.00	2.08
GLU69	HG3	1.00	0.010	1.00	1.15
GLU69	H	1.00	0.012	1.00	-1383855.00
LEU70	HA	1.00	0.316	0.00	0.00
LEU70	H	1.00	0.008	1.00	-497468.00

3.69.6 Detailed Probabilities of GLU69HB2:

Overall probability: 0.486

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU69	0.40	0.86
LEU70	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E69HA	1.00
E69HB3	1.00
E69HG2	1.00
E69HG3	1.00
E69H	1.00
E69HE2	1.00
E69HB2	1.00
L70H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU69	HA	1.00	0.036	0.40	0.00
GLU69	HB2	1.00	0.019	1.00	19.33
GLU69	HB3	1.00	0.079	0.00	0.00
GLU69	HG2	1.00	0.095	0.00	0.00
GLU69	HG3	1.00	0.082	0.00	0.00
GLU69	H	1.00	0.000	1.00	-1353797.00
LEU70	H	1.00	0.002	1.00	-621522.00

3.69.7 Detailed Probabilities of GLU69HB3:

Overall probability: 0.900

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU69	0.88	0.86
LEU70	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E69HA	1.00
E69HB2	1.00
E69HG2	1.00
E69HG3	1.00
E69H	1.00
E69HE2	1.00
E69HB3	1.00
L70H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU69	HA	1.00	0.011	1.00	5.05
GLU69	HB2	1.00	0.033	0.70	0.00
GLU69	HB3	1.00	0.004	1.00	35.26
GLU69	HG2	1.00	0.009	1.00	8.87
GLU69	HG3	1.00	0.002	1.00	3.11
GLU69	H	1.00	0.034	0.60	0.00
LEU70	H	1.00	0.010	1.00	-705333.00

3.69.8 Detailed Probabilities of GLU69HG2:

Overall probability: 0.574

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU69	0.67	0.86
LEU70	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
E69HA	1.00
E69HB2	1.00
E69HB3	1.00
E69HG3	1.00
E69H	1.00
E69HE2	1.00
E69HG2	1.00
L70H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU69	HA	1.00	0.009	1.00	2.14
GLU69	HB2	1.00	0.077	0.00	0.00
GLU69	HB3	1.00	0.007	1.00	3.87
GLU69	HG2	1.00	0.023	1.00	100.68
GLU69	HG3	1.00	0.010	1.00	6.47
GLU69	H	1.00	0.072	0.00	0.00
LEU70	H	0.98	0.074	0.02	0.00

3.69.9 Detailed Probabilities of GLU69HG3:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU69	1.00	0.86
LEU70	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E69HA	1.00
E69HB2	1.00
E69HB3	1.00
E69HG2	1.00
E69H	1.00
E69HE2	1.00
E69HG3	1.00
L70H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU69	HA	1.00	0.013	1.00	1.54
GLU69	HB2	1.00	0.024	1.00	2.85
GLU69	HB3	1.00	0.007	1.00	2.04
GLU69	HG2	1.00	0.008	1.00	7.48
GLU69	HG3	1.00	0.008	1.00	35.10
GLU69	H	1.00	0.001	1.00	-613247.00
LEU70	H	0.97	0.012	1.00	-163332.00

3.69.10 Detailed Probabilities of GLU69H:

Overall probability: 0.848

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU68	0.86	1.00
GLU69	0.95	1.00
LEU70	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
L68HA	1.00
L68HB2	1.00
L68HB3	1.00
L68HG	0.98
L68H	1.00
E69HA	1.00
E69HB2	1.00
E69HB3	1.00
E69HG2	1.00
E69HG3	1.00
E69H	1.00
L70H	1.00

NOESY contacts detailed probability

3.69 GLU(69)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU68	HA	1.00	0.015	1.00	0.14
LEU68	HB2	1.00	0.008	1.00	0.53
LEU68	HB3	1.00	0.015	1.00	0.66
LEU68	HG	0.98	0.618	0.02	0.00
LEU68	H	1.00	0.007	1.00	-758646.00
LEU68	HD11	0.51	0.015	1.00	0.09
LEU68	HD21	0.58	0.013	1.00	0.09
GLU69	HA	1.00	0.001	1.00	0.91
GLU69	HB2	1.00	0.005	1.00	0.92
GLU69	HB3	1.00	0.033	0.70	0.00
GLU69	HG2	1.00	0.003	1.00	0.51
GLU69	HG3	1.00	0.008	1.00	0.71
GLU69	H	1.00	0.017	1.00	-19107776.00
LEU70	H	1.00	0.100	0.00	0.00
LEU70	HB2	0.69	0.023	1.00	0.29

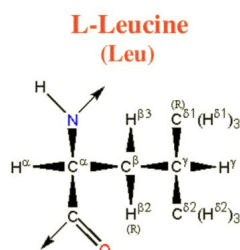
3.70 LEU(70)

Figure 69: Image from the BMRB

Residue probability: 0.719

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	179.699	177.056	1.929	0.000	0.000
CA 3.70.1	57.774	55.735	3.802	0.545	1.000
CB 3.70.2	41.944	42.389	3.750	0.875	1.000
CG 3.70.3	26.770	26.892	3.086	0.500	1.000
CD1 3.70.4	25.175	24.837	3.657	0.857	1.000
CD2 3.70.5	23.168	24.201	3.117	0.757	1.000
N 3.70.6	119.503	121.785	4.943	0.868	1.000
HA 3.70.7	4.161	4.315	0.840	0.727	1.000
HB2 3.70.8	1.942	1.601	0.373	0.375	1.000
HB3 3.70.9	1.570	1.508	0.398	0.700	1.000
HG 3.70.10	1.848	1.510	0.340	0.502	1.000
HD1 3.70.11	0.906	0.739	0.294	0.857	1.000
HD2 3.70.12	0.903	0.727	0.421	0.857	1.000
H 3.70.13	7.717	8.237	0.647	0.931	1.000

3.70.1 Detailed Probabilities of LEU70CA:

Overall probability: 0.545

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU69	0.00	1.00
LEU70	0.43	1.00
ILE71	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E69HA	1.00
L70HB2	1.00
L70HB3	1.00
L70HG	1.00
L70HD11	0.99
L70HD21	0.99
L70H	1.00
L70HA	1.00
I71H	1.00
I71HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU69	HA	1.00	0.316	0.00	0.00
LEU70	HA	1.00	0.422	0.00	0.00
LEU70	HB2	1.00	0.041	0.00	0.00
LEU70	HB3	1.00	0.078	0.00	0.00
LEU70	HG	1.00	0.053	0.00	0.00
LEU70	HD11	0.99	0.000	1.00	1.97
LEU70	HD21	0.99	0.003	1.00	1.97
LEU70	H	1.00	0.009	1.00	0.62
ILE71	HA	1.00	0.002	1.00	0.07
ILE71	H	1.00	0.006	1.00	0.20
ILE71	HG13	0.63	0.001	1.00	0.08

3.70.2 Detailed Probabilities of LEU70CB:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU70	0.86	1.00
ILE71	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L70HA	1.00
L70HB3	1.00
L70HG	1.00
L70HD11	1.00
L70HD21	1.00
L70H	1.00
L70HB2	1.00
I71H	1.00

NOESY contacts detailed probability

3.70 LEU(70)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU70	HA	1.00	0.001	1.00	0.74
LEU70	HB2	1.00	0.016	1.00	5.90
LEU70	HB3	1.00	0.028	1.00	3.74
LEU70	HG	1.00	0.078	0.00	0.00
LEU70	HD11	1.00	0.008	1.00	1.66
LEU70	HD21	1.00	0.011	1.00	1.66
LEU70	H	1.00	0.011	1.00	0.62
ILE71	H	1.00	0.008	1.00	0.24

3.70.3 Detailed Probabilities of LEU70CG:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU70	0.43	1.00
ILE71	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L70HA	1.00
L70HB2	1.00
L70HB3	1.00
L70HD11	1.00
L70HD21	1.00
L70H	1.00
L70HG	1.00
I71H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU70	HA	1.00	0.085	0.00	0.00
LEU70	HB2	1.00	0.071	0.00	0.00
LEU70	HB3	1.00	0.025	1.00	0.88
LEU70	HG	1.00	0.023	1.00	12.24
LEU70	HD11	1.00	0.401	0.00	0.00
LEU70	HD21	1.00	0.404	0.00	0.00
LEU70	H	1.00	0.012	1.00	0.78
ILE71	H	0.99	0.006	1.00	0.08

3.70.4 Detailed Probabilities of LEU70CD1:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU70	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
L70HA	0.99
L70HB2	1.00
L70HB3	1.00
L70HG	1.00
L70HD12	1.00
L70HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU70	HA	0.99	0.024	1.00	0.42
LEU70	HB2	1.00	0.005	1.00	1.37
LEU70	HB3	1.00	0.061	0.00	0.00
LEU70	HG	1.00	0.009	1.00	2.01
LEU70	HD11	1.00	0.004	1.00	147.68
LEU70	HD21	1.00	0.001	1.00	147.68
LEU70	H	0.86	0.015	1.00	0.31

3.70.5 Detailed Probabilities of LEU70CD2:

Overall probability: 0.757

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU70	0.76	1.00

Expected NOESY Contacts

Proton	Expected probability
L70HA	0.99
L70HB2	1.00
L70HB3	1.00
L70HG	1.00
L70HD11	1.00
L70HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU70	HA	0.99	0.002	1.00	2.12
LEU70	HB2	1.00	0.093	0.00	0.00
LEU70	HB3	1.00	0.037	0.30	0.00
LEU70	HG	1.00	0.001	1.00	2.84
LEU70	HD11	1.00	0.026	1.00	78.89
LEU70	HD21	1.00	0.029	1.00	78.89
LEU70	H	0.85	0.010	1.00	0.48

3.70.6 Detailed Probabilities of LEU70N:

Overall probability: 0.868

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU69	0.67	1.00
LEU70	1.00	1.00
ILE71	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E69HB2	1.00
E69HG2	0.98
E69HG3	0.97
E69HB3	1.00
E69H	1.00
E69HA	1.00
L70HA	1.00
L70HB2	1.00
L70HB3	1.00
L70HG	1.00
L70H	1.00
I71H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU69	HA	1.00	0.008	1.00	-497468.00
GLU69	HB2	1.00	0.002	1.00	-621522.00
GLU69	HB3	1.00	0.010	1.00	-705333.00
GLU69	HG2	0.98	0.074	0.02	0.00
GLU69	HG3	0.97	0.012	1.00	-163332.00
GLU69	H	1.00	0.100	0.00	0.00
LEU70	HA	1.00	0.004	1.00	-772485.00
LEU70	HB2	1.00	0.010	1.00	-1305406.00
LEU70	HB3	1.00	0.009	1.00	-1001450.00
LEU70	HG	1.00	0.001	1.00	-1268251.00
LEU70	H	1.00	0.010	1.00	-9151724.00
LEU70	HD11	0.88	0.000	1.00	-895818.00
LEU70	HD21	0.87	0.003	1.00	-895818.00
ILE71	H	1.00	0.008	1.00	-823522.00
ILE71	HA	0.93	0.029	1.00	-167917.00

3.70.7 Detailed Probabilities of LEU70HA:

Overall probability: 0.727

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU69	0.50	1.00
LEU70	0.71	1.00
ILE71	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E69HA	1.00
L70HB2	1.00
L70HB3	1.00
L70HG	1.00
L70HD11	0.99
L70HD21	0.99
L70H	1.00
L70HA	1.00
I71H	1.00
I71HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU69	HA	1.00	0.119	0.00	0.00
GLU69	HB2	0.68	0.027	1.00	0.58
LEU70	HA	1.00	0.422	0.00	0.00
LEU70	HB2	1.00	0.001	1.00	0.74
LEU70	HB3	1.00	0.002	1.00	0.64
LEU70	HG	1.00	0.085	0.00	0.00
LEU70	HD11	0.99	0.024	1.00	0.42
LEU70	HD21	0.99	0.002	1.00	2.12
LEU70	H	1.00	0.004	1.00	-772485.00
ILE71	HA	1.00	0.012	1.00	0.05
ILE71	H	1.00	0.002	1.00	-195698.00

3.70.8 Detailed Probabilities of LEU70HB2:

Overall probability: 0.375

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU70	0.43	1.00
ILE71	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L70HA	1.00
L70HB3	1.00
L70HG	1.00
L70HD11	1.00
L70HD21	1.00
L70H	1.00
L70HB2	1.00
I71H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU70	HA	1.00	0.041	0.00	0.00
LEU70	HB2	1.00	0.016	1.00	5.90
LEU70	HB3	1.00	0.118	0.00	0.00
LEU70	HG	1.00	0.071	0.00	0.00
LEU70	HD11	1.00	0.005	1.00	1.37
LEU70	HD21	1.00	0.093	0.00	0.00
LEU70	H	1.00	0.010	1.00	-1305406.00
ILE71	H	1.00	0.040	0.00	0.00

3.70.9 Detailed Probabilities of LEU70HB3:

Overall probability: 0.700

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU70	0.61	1.00
ILE71	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L70HA	1.00
L70HB2	1.00
L70HG	1.00
L70HD11	1.00
L70HD21	1.00
L70H	1.00
L70HB3	1.00
I71H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU70	HA	1.00	0.078	0.00	0.00
LEU70	HB2	1.00	0.028	1.00	3.74
LEU70	HB3	1.00	0.018	1.00	8.63
LEU70	HG	1.00	0.025	1.00	0.88
LEU70	HD11	1.00	0.061	0.00	0.00
LEU70	HD21	1.00	0.037	0.30	0.00
LEU70	H	1.00	0.009	1.00	-1001450.00
ILE71	H	1.00	0.004	1.00	-295135.00
ILE71	HA	0.92	0.009	1.00	0.09

3.70.10 Detailed Probabilities of LEU70HG:

Overall probability: 0.502

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU70	0.57	1.00
ILE71	0.01	1.00

Expected NOESY Contacts

Proton	Expected probability
L70HA	1.00
L70HB2	1.00
L70HB3	1.00
L70HD11	1.00
L70HD21	1.00
L70H	1.00
L70HG	1.00
I71H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU70	HA	1.00	0.053	0.00	0.00
LEU70	HB2	1.00	0.078	0.00	0.00
LEU70	HB3	1.00	0.212	0.00	0.00
LEU70	HG	1.00	0.023	1.00	12.24
LEU70	HD11	1.00	0.009	1.00	2.01
LEU70	HD21	1.00	0.001	1.00	2.84
LEU70	H	1.00	0.001	1.00	-1268251.00
ILE71	H	0.99	0.054	0.01	0.00

3.70.11 Detailed Probabilities of LEU70HD11:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU70	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
L70HA	0.99
L70HB2	1.00
L70HB3	1.00
L70HG	1.00
L70HD12	1.00
L70HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU70	HA	0.99	0.000	1.00	1.97
LEU70	HB2	1.00	0.008	1.00	1.66
LEU70	HB3	1.00	0.005	1.00	1.80
LEU70	HG	1.00	0.401	0.00	0.00
LEU70	HD11	1.00	0.004	1.00	147.68
LEU70	HD21	1.00	0.026	1.00	78.89
LEU70	H	0.86	0.000	1.00	-895818.00

3.70.12 Detailed Probabilities of LEU70HD21:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU70	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
L70HA	0.99
L70HB2	1.00
L70HB3	1.00
L70HG	1.00
L70HD11	1.00
L70HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU70	HA	0.99	0.003	1.00	1.97
LEU70	HB2	1.00	0.011	1.00	1.66
LEU70	HB3	1.00	0.008	1.00	1.80
LEU70	HG	1.00	0.404	0.00	0.00
LEU70	HD11	1.00	0.001	1.00	147.68
LEU70	HD21	1.00	0.029	1.00	78.89
LEU70	H	0.85	0.003	1.00	-895818.00

3.70.13 Detailed Probabilities of LEU70H:

Overall probability: 0.931

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU69	0.82	1.00
LEU70	1.00	1.00
ILE71	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E69HB2	1.00
E69HG2	0.98
E69HG3	0.97
E69HB3	1.00
E69H	1.00
E69HA	1.00
L70HA	1.00
L70HB2	1.00
L70HB3	1.00
L70HG	1.00
L70H	1.00
I71H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU69	HA	1.00	0.085	0.00	0.00
GLU69	HB2	1.00	0.011	1.00	0.38
GLU69	HB3	1.00	0.017	1.00	0.71
GLU69	HG2	0.98	0.007	1.00	0.52
GLU69	HG3	0.97	0.014	1.00	0.17
GLU69	H	1.00	0.031	0.90	0.00
LEU70	HA	1.00	0.009	1.00	0.62
LEU70	HB2	1.00	0.011	1.00	0.62
LEU70	HB3	1.00	0.010	1.00	0.53
LEU70	HG	1.00	0.012	1.00	0.78
LEU70	H	1.00	0.010	1.00	-9151724.00
LEU70	HD11	0.88	0.015	1.00	0.31
LEU70	HD21	0.87	0.010	1.00	0.48
ILE71	H	1.00	0.010	1.00	-668664.00
ILE71	HA	0.93	0.011	1.00	0.09
ILE71	HB	0.52	0.009	1.00	0.06

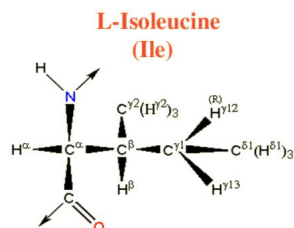


Figure 70: Image from the BMRB

Residue probability: 0.802
 Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.357	175.926	2.710	0.000	0.000
CA 3.71.1	64.242	61.717	4.152	0.923	1.000
CB 3.71.2	37.901	38.702	3.945	1.000	1.000
CG1 3.71.3	28.690	27.785	2.037	0.875	1.000
CG2 3.71.4	18.372	17.574	1.928	0.445	1.000
CD1 3.71.5	14.719	13.545	3.646	0.643	1.000
N 3.71.6	116.791	121.467	6.098	0.868	1.000
HA 3.71.7	3.737	4.185	1.403	0.885	1.000
HB 3.71.8	1.896	1.776	0.310	0.750	1.000
HG12 3.71.9	1.693	1.271	0.411	0.875	1.000
HG13 3.71.10	1.022	1.186	0.426	0.625	1.000
HG2 3.71.11	0.817	0.762	0.283	0.889	1.000
HD1 3.71.12	0.654	0.668	0.293	0.715	1.000
H 3.71.13	8.598	8.301	0.685	0.933	1.000

3.71.1 Detailed Probabilities of ILE71CA:

Overall probability: 0.923
 Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU70	1.00	1.00
ILE71	1.00	1.00
SER72	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
L70HA	1.00
I71HB	1.00
I71HG12	1.00
I71HG13	1.00
I71HG21	1.00
I71HD11	0.97
I71H	1.00
I71HA	1.00
S72HA	1.00
S72H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU70	HA	1.00	0.012	1.00	0.05
LEU70	HB3	0.92	0.009	1.00	0.09
LEU70	H	0.93	0.011	1.00	0.09
ILE71	HA	1.00	0.006	1.00	4.18
ILE71	HB	1.00	0.002	1.00	0.50
ILE71	HG12	1.00	0.014	1.00	0.56
ILE71	HG13	1.00	0.001	1.00	0.28
ILE71	HG21	1.00	0.004	1.00	1.44
ILE71	HD11	0.97	0.002	1.00	0.26
ILE71	H	1.00	0.011	1.00	0.32
SER72	HA	1.00	0.216	0.00	0.00
SER72	H	1.00	0.001	1.00	0.14
SER72	HB2	0.54	0.027	1.00	0.05

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
SER72	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
S72H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE71	HA	1.00	0.024	1.00	0.55
ILE71	HB	1.00	0.016	1.00	3.48
ILE71	HG12	1.00	0.022	1.00	0.55
ILE71	HG13	1.00	0.002	1.00	0.27
ILE71	HG21	1.00	0.022	1.00	1.61
ILE71	HD11	1.00	0.003	1.00	0.79
ILE71	H	1.00	0.011	1.00	0.50
SER72	H	1.00	0.006	1.00	0.17

3.71.3 Detailed Probabilities of ILE71CG1:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE71	0.86	1.00
SER72	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
S72H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE71	HA	1.00	0.024	1.00	0.25
ILE71	HB	1.00	0.212	0.00	0.00
ILE71	HG12	1.00	0.009	1.00	244.35
ILE71	HG13	1.00	0.002	1.00	0.75
ILE71	HG21	1.00	0.005	1.00	0.62
ILE71	HD11	1.00	0.008	1.00	0.74
ILE71	H	1.00	0.006	1.00	0.26
SER72	H	0.98	0.004	1.00	0.12

3.71.4 Detailed Probabilities of ILE71CG2:

Overall probability: 0.445

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE71	0.29	1.00
SER72	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
S72H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE71	HA	1.00	0.014	1.00	1.00
ILE71	HB	1.00	0.064	0.00	0.00
ILE71	HG12	1.00	0.016	1.00	0.57
ILE71	HG13	1.00	0.495	0.00	0.00
ILE71	HG21	1.00	0.290	0.00	0.00
ILE71	HD11	0.99	0.127	0.01	0.00
ILE71	H	1.00	0.049	0.00	0.00
SER72	H	0.98	0.029	1.00	0.17
SER72	HA	0.58	0.003	1.00	0.15

3.71.5 Detailed Probabilities of ILE71CD1:

Overall probability: 0.643

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE71	0.64	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	0.035	0.50	0.00
ILE71	HB	1.00	0.006	1.00	0.93
ILE71	HG12	1.00	0.120	0.00	0.00
ILE71	HG13	1.00	0.110	0.00	0.00
ILE71	HG21	0.99	0.004	1.00	2.00
ILE71	HD11	1.00	0.004	1.00	28.01
ILE71	H	0.94	0.011	1.00	0.31

3.71.6 Detailed Probabilities of ILE71N:

Overall probability: 0.868

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU70	0.72	1.00
ILE71	1.00	1.00
SER72	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L70HB2	1.00
L70H	1.00
L70HB3	1.00
L70HA	1.00
L70HG	0.99
I71HA	1.00
I71HB	1.00
I71HG12	1.00
I71HG13	1.00
I71HG21	1.00
I71H	1.00
S72H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU70	HA	1.00	0.002	1.00	-195698.00
LEU70	HB2	1.00	0.040	0.00	0.00
LEU70	HB3	1.00	0.004	1.00	-295135.00
LEU70	HG	0.99	0.054	0.01	0.00
LEU70	H	1.00	0.010	1.00	-668664.00
LEU70	HD11	0.53	0.006	1.00	-197180.00
LEU70	HD21	0.63	0.009	1.00	-197180.00
ILE71	HA	1.00	0.015	1.00	-525321.00
ILE71	HB	1.00	0.006	1.00	-820664.00
ILE71	HG12	1.00	0.011	1.00	-575538.00
ILE71	HG13	1.00	0.004	1.00	-398103.00
ILE71	HG21	1.00	0.001	1.00	-484428.00
ILE71	H	1.00	0.008	1.00	-3508449.00
ILE71	HD11	0.94	0.011	1.00	-346274.00
SER72	H	1.00	0.002	1.00	-442658.00

3.71.7 Detailed Probabilities of ILE71HA:

Overall probability: 0.885

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU70	1.00	1.00
ILE71	0.93	1.00
SER72	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
L70HA	1.00
I71HB	1.00
I71HG12	1.00
I71HG13	1.00
I71HG21	1.00
I71HD11	0.97
I71H	1.00
I71HA	1.00
S72HA	1.00
S72H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU70	HA	1.00	0.002	1.00	0.07
LEU70	HB3	0.92	0.015	1.00	0.06
LEU70	H	0.93	0.029	1.00	-167917.00
ILE71	HA	1.00	0.006	1.00	4.18
ILE71	HB	1.00	0.024	1.00	0.55
ILE71	HG12	1.00	0.024	1.00	0.25
ILE71	HG13	1.00	0.021	1.00	0.29
ILE71	HG21	1.00	0.014	1.00	1.00
ILE71	HD11	0.97	0.035	0.50	0.00
ILE71	H	1.00	0.015	1.00	-525321.00
SER72	HA	1.00	0.137	0.00	0.00
SER72	H	1.00	0.016	1.00	-332628.00
SER72	HB2	0.54	0.028	1.00	0.09

3.71.8 Detailed Probabilities of ILE71HB:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE71	0.71	1.00
SER72	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
S72H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE71	HA	1.00	0.002	1.00	0.50
ILE71	HB	1.00	0.016	1.00	3.48
ILE71	HG12	1.00	0.212	0.00	0.00
ILE71	HG13	1.00	0.008	1.00	0.24
ILE71	HG21	1.00	0.064	0.00	0.00
ILE71	HD11	1.00	0.006	1.00	0.93
ILE71	H	1.00	0.006	1.00	-820664.00
SER72	H	1.00	0.002	1.00	-480652.00

3.71.9 Detailed Probabilities of ILE71HG12:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE71	0.86	1.00
SER72	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
S72H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE71	HA	1.00	0.014	1.00	0.56
ILE71	HB	1.00	0.022	1.00	0.55
ILE71	HG12	1.00	0.009	1.00	244.35
ILE71	HG13	1.00	0.014	1.00	0.79
ILE71	HG21	1.00	0.016	1.00	0.57
ILE71	HD11	1.00	0.120	0.00	0.00
ILE71	H	1.00	0.011	1.00	-575538.00
SER72	H	0.98	0.011	1.00	-252379.00

3.71.10 Detailed Probabilities of ILE71HG13:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE71	0.57	1.00
SER72	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
S72H	0.95

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE71	HA	1.00	0.001	1.00	0.28
ILE71	HB	1.00	0.002	1.00	0.27
ILE71	HG12	1.00	0.002	1.00	0.75
ILE71	HG13	1.00	0.201	0.00	0.00
ILE71	HG21	1.00	0.495	0.00	0.00
ILE71	HD11	1.00	0.110	0.00	0.00
ILE71	H	1.00	0.004	1.00	-398103.00
SER72	H	0.95	0.003	1.00	-135564.00

3.71.11 Detailed Probabilities of ILE71HG21:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE71	0.86	1.00
SER72	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
S72H	0.98

NOESY contacts detailed probability

3.71 ILE(71)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE71	HA	1.00	0.004	1.00	1.44
ILE71	HB	1.00	0.022	1.00	1.61
ILE71	HG12	1.00	0.005	1.00	0.62
ILE71	HG13	1.00	0.004	1.00	0.30
ILE71	HG21	1.00	0.290	0.00	0.00
ILE71	HD11	0.99	0.004	1.00	2.00
ILE71	H	1.00	0.001	1.00	-484428.00
SER72	H	0.98	0.001	1.00	-381463.00
SER72	HA	0.58	0.000	1.00	0.17

3.71.12 Detailed Probabilities of ILE71HD11:

Overall probability: 0.715

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE71	0.72	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	0.002	1.00	0.26
ILE71	HB	1.00	0.003	1.00	0.79
ILE71	HG12	1.00	0.008	1.00	0.74
ILE71	HG13	1.00	0.167	0.00	0.00
ILE71	HG21	0.99	0.127	0.01	0.00
ILE71	HD11	1.00	0.004	1.00	28.01
ILE71	H	0.94	0.011	1.00	-346274.00

3.71.13 Detailed Probabilities of ILE71H:

Overall probability: 0.933

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU70	1.00	1.00
ILE71	0.86	1.00
SER72	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L70HB2	1.00
L70H	1.00
L70HB3	1.00
L70HA	1.00
L70HG	0.99
I71HA	1.00
I71HB	1.00
I71HG12	1.00
I71HG13	1.00
I71HG21	1.00
I71H	1.00
S72H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU70	HA	1.00	0.006	1.00	0.20
LEU70	HB2	1.00	0.008	1.00	0.24
LEU70	HB3	1.00	0.010	1.00	0.21
LEU70	HG	0.99	0.006	1.00	0.08
LEU70	H	1.00	0.008	1.00	-823522.00
LEU70	HD11	0.53	0.008	1.00	0.33
LEU70	HD21	0.63	0.001	1.00	0.10
ILE71	HA	1.00	0.011	1.00	0.32
ILE71	HB	1.00	0.011	1.00	0.50
ILE71	HG12	1.00	0.006	1.00	0.26
ILE71	HG13	1.00	0.008	1.00	0.24
ILE71	HG21	1.00	0.049	0.00	0.00
ILE71	H	1.00	0.008	1.00	-3508449.00
ILE71	HD11	0.94	0.011	1.00	0.31
SER72	H	1.00	0.007	1.00	-710434.00

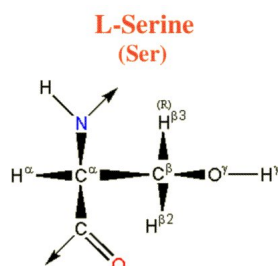


Figure 71: Image from the BMRB

Residue probability: 0.762
Residue probability confidence: 0.855

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	176.845	174.682	1.868	0.000	0.000
CA 3.72.1	61.365	58.750	3.025	0.429	0.857
CB 3.72.2	62.780	63.523	4.288	1.000	0.800
N 3.72.3	116.517	116.135	5.326	1.000	0.909
HA 3.72.4	4.365	4.486	0.430	0.571	0.857
HB 3.72.5	4.122	3.856	0.325	0.750	0.800
H 3.72.6	8.023	8.292	0.600	0.822	0.909
HG	NA	—	—	0.000	0.000

3.72.1 Detailed Probabilities of SER72CA:

Overall probability: 0.429
Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE71	0.50	1.00
SER72	0.33	0.75
LYS73	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
I71HA	1.00
S72HB2	1.00
S72H	1.00
S72HG	1.00
S72HA	1.00
K73HA	1.00
K73H	1.00

NOESY contacts detailed probability

3.72 SER(72)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE71	HA	1.00	0.137	0.00	0.00
ILE71	HG21	0.61	0.000	1.00	0.17
SER72	HA	1.00	0.002	1.00	7.76
SER72	HB2	1.00	0.245	0.00	0.00
SER72	H	1.00	0.303	0.00	0.00
LYS73	HA	1.00	0.076	0.00	0.00
LYS73	H	1.00	0.003	1.00	0.20

3.72.2 Detailed Probabilities of SER72CB:

Overall probability: 1.000

Overall confidence: 0.800

Inter- and intra-residue probability

Residue	Probability	Confidence
SER72	1.00	0.75
LYS73	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S72HA	1.00
S72HB3	1.00
S72H	1.00
S72HG	1.00
K73H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER72	HA	1.00	0.001	1.00	0.76
SER72	HB2	1.00	0.001	1.00	15.35
SER72	H	1.00	0.009	1.00	0.84
LYS73	H	1.00	0.007	1.00	0.21

3.72.3 Detailed Probabilities of SER72N:

Overall probability: 1.000

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE71	1.00	1.00
SER72	1.00	0.75
LYS73	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I71H	1.00
I71HB	1.00
I71HG12	0.98
I71HG13	0.95
I71HA	1.00
I71HG22	0.98
S72HA	1.00
S72HB2	1.00
S72HG	1.00
S72H	1.00
K73H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE71	HA	1.00	0.016	1.00	-332628.00
ILE71	HB	1.00	0.002	1.00	-480652.00
ILE71	HG12	0.98	0.011	1.00	-252379.00
ILE71	HG13	0.95	0.003	1.00	-135564.00
ILE71	HG21	0.98	0.001	1.00	-381463.00
ILE71	H	1.00	0.007	1.00	-710434.00
SER72	HA	1.00	0.001	1.00	-706490.00
SER72	HB2	1.00	0.004	1.00	-1258446.00
SER72	H	1.00	0.004	1.00	-7597338.00
LYS73	H	1.00	0.001	1.00	-644280.00
LYS73	HB2	0.50	0.001	1.00	-480652.00

3.72.4 Detailed Probabilities of SER72HA:

Overall probability: 0.571

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE71	0.50	1.00
SER72	1.00	0.75
LYS73	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I71HA	1.00
S72HB2	1.00
S72H	1.00
S72HG	1.00
S72HA	1.00
K73HA	1.00
K73H	1.00

NOESY contacts detailed probability

3.72 SER(72)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE71	HA	1.00	0.216	0.00	0.00
ILE71	HG21	0.61	0.003	1.00	0.15
SER72	HA	1.00	0.002	1.00	7.76
SER72	HB2	1.00	0.001	1.00	0.76
SER72	H	1.00	0.001	1.00	-706490.00
LYS73	HA	1.00	0.083	0.00	0.00
LYS73	H	1.00	0.060	0.00	0.00

3.72.5 Detailed Probabilities of SER72HB2:

Overall probability: 0.750

Overall confidence: 0.800

Inter- and intra-residue probability

Residue	Probability	Confidence
SER72	0.67	0.75
LYS73	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S72HA	1.00
S72HB3	1.00
S72H	1.00
S72HG	1.00
K73H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER72	HA	1.00	0.245	0.00	0.00
SER72	HB2	1.00	0.001	1.00	15.35
SER72	H	1.00	0.004	1.00	-1258446.00
LYS73	H	1.00	0.008	1.00	-457591.00

3.72.6 Detailed Probabilities of SER72H:

Overall probability: 0.822

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE71	0.84	1.00
SER72	0.67	0.75
LYS73	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I71H	1.00
I71HB	1.00
I71HG12	0.98
I71HG13	0.95
I71HA	1.00
I71HG22	0.98
S72HA	1.00
S72HB2	1.00
S72HG	1.00
S72H	1.00
K73H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE71	HA	1.00	0.001	1.00	0.14
ILE71	HB	1.00	0.006	1.00	0.17
ILE71	HG12	0.98	0.004	1.00	0.12
ILE71	HG13	0.95	0.583	0.05	0.00
ILE71	HG21	0.98	0.029	1.00	0.17
ILE71	H	1.00	0.002	1.00	-442658.00
SER72	HA	1.00	0.303	0.00	0.00
SER72	HB2	1.00	0.009	1.00	0.84
SER72	H	1.00	0.004	1.00	-7597338.00
LYS73	H	1.00	0.005	1.00	-549382.00
LYS73	HB2	0.50	0.008	1.00	1.13

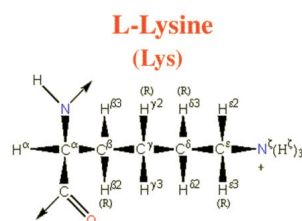


Figure 72: Image from the BMRB

Residue probability: 0.845
Residue probability confidence: 0.932

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	177.771	176.660	3.133	0.000	0.000
CA 3.73.1	57.476	57.014	3.028	0.846	1.000
CB 3.73.2	32.146	32.981	3.186	0.802	1.000
CG 3.73.3	24.910	24.941	1.956	0.980	0.909
CD 3.73.4	28.780	29.020	2.193	0.750	0.900
CE 3.73.5	41.780	41.893	1.492	0.878	0.889
N 3.73.6	120.731	120.954	4.210	0.923	0.909
NZ	NA	—	—	0.000	0.000
HA 3.73.7	4.291	4.262	0.489	0.769	1.000
HB2 3.73.8	1.895	1.774	0.365	0.782	1.000
HB3 3.73.9	1.894	1.742	0.385	0.745	1.000
HG2 3.73.10	1.597	1.358	0.344	0.730	0.917
HG3 3.73.11	1.478	1.343	0.357	1.000	0.909
HD2 3.73.12	1.684	1.614	0.957	0.900	0.900
HD3 3.73.13	1.683	1.595	0.387	0.900	0.900
HE2 3.73.14	2.982	2.907	0.230	0.781	0.889
HE3 3.73.15	2.977	2.901	0.241	0.780	0.889
H 3.73.16	7.723	8.185	0.605	0.954	0.909
HZ	NA	—	—	0.000	0.000

3.73.1 Detailed Probabilities of LYS73CA:

Overall probability: 0.846
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
SER72	0.00	1.00
LYS73	1.00	1.00
LEU74	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
S72HA	1.00
K73HB2	1.00
K73HB3	1.00
K73HG2	1.00
K73HG3	1.00
K73HD2	0.98
K73HD3	0.98
K73H	1.00
K73HA	1.00
L74HA	1.00
L74H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER72	HA	1.00	0.083	0.00	0.00
LYS73	HA	1.00	0.009	1.00	12.17
LYS73	HB2	1.00	0.024	1.00	2.01
LYS73	HB3	1.00	0.025	1.00	2.01
LYS73	HG2	1.00	0.017	1.00	0.46
LYS73	HG3	1.00	0.010	1.00	0.74
LYS73	HD2	0.98	0.002	1.00	0.52
LYS73	HD3	0.98	0.003	1.00	0.52
LYS73	H	1.00	0.001	1.00	0.66
LYS73	HE2	0.77	0.009	1.00	0.06
LYS73	HE3	0.76	0.014	1.00	0.06
LEU74	HA	1.00	0.055	0.00	0.00
LEU74	H	1.00	0.006	1.00	0.38

3.73.2 Detailed Probabilities of LYS73CB:

Overall probability: 0.802

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS73	0.78	1.00
LEU74	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K73HA	1.00
K73HB3	1.00
K73HG2	1.00
K73HG3	1.00
K73HD2	1.00
K73HD3	1.00
K73HE2	0.98
K73HE3	0.99
K73H	1.00
K73HB2	1.00
L74H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS73	HA	1.00	0.015	1.00	1.59
LYS73	HB2	1.00	0.009	1.00	53.87
LYS73	HB3	1.00	0.010	1.00	53.87
LYS73	HG2	1.00	0.014	1.00	3.20
LYS73	HG3	1.00	0.005	1.00	3.41
LYS73	HD2	1.00	0.001	1.00	5.56
LYS73	HD3	1.00	0.000	1.00	5.56
LYS73	HE2	0.98	0.053	0.02	0.00
LYS73	HE3	0.99	0.048	0.01	0.00
LYS73	H	1.00	0.032	0.80	0.00
LEU74	H	1.00	0.006	1.00	2.14

3.73.3 Detailed Probabilities of LYS73CG:

Overall probability: 0.980

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS73	0.98	0.91

Expected NOESY Contacts

Proton	Expected probability
K73HA	1.00
K73HB2	1.00
K73HB3	1.00
K73HG2	1.00
K73HD2	1.00
K73HD3	1.00
K73HE2	1.00
K73HE3	1.00
K73H	1.00
K73HZ2	1.00
K73HG3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS73	HA	1.00	0.024	1.00	0.81
LYS73	HB2	1.00	0.003	1.00	2.94
LYS73	HB3	1.00	0.002	1.00	2.94
LYS73	HG2	1.00	0.007	1.00	6.42
LYS73	HG3	1.00	0.009	1.00	52.13
LYS73	HD2	1.00	0.002	1.00	6.34
LYS73	HD3	1.00	0.001	1.00	6.34
LYS73	HE2	1.00	0.022	1.00	0.86
LYS73	HE3	1.00	0.017	1.00	0.86
LYS73	H	1.00	0.032	0.80	0.00

3.73.4 Detailed Probabilities of LYS73CD:

Overall probability: 0.750

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS73	0.75	0.90

Expected NOESY Contacts

Proton	Expected probability
K73HA	0.98
K73HB2	1.00
K73HB3	1.00
K73HG2	1.00
K73HG3	1.00
K73HD3	1.00
K73HE2	1.00
K73HE3	1.00
K73HZ2	1.00
K73HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS73	HA	0.98	0.020	1.00	1.05
LYS73	HB2	1.00	0.037	0.30	0.00
LYS73	HB3	1.00	0.038	0.20	0.00
LYS73	HG2	1.00	0.087	0.00	0.00
LYS73	HG3	1.00	0.019	1.00	11.42
LYS73	HD2	1.00	0.000	1.00	244.35
LYS73	HD3	1.00	0.001	1.00	244.35
LYS73	HE2	1.00	0.000	1.00	6.07
LYS73	HE3	1.00	0.005	1.00	6.07
LYS73	H	0.87	0.002	1.00	0.35

3.73.5 Detailed Probabilities of LYS73CE:

Overall probability: 0.878

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS73	0.88	0.89

Expected NOESY Contacts

Proton	Expected probability
K73HB2	0.98
K73HB3	0.99
K73HG2	1.00
K73HG3	1.00
K73HD2	1.00
K73HD3	1.00
K73HE3	1.00
K73HZ2	1.00
K73HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS73	HB2	0.98	0.035	0.50	0.00
LYS73	HB3	0.99	0.036	0.40	0.00
LYS73	HG2	1.00	0.010	1.00	2.64
LYS73	HG3	1.00	0.014	1.00	3.64
LYS73	HD2	1.00	0.012	1.00	15.02
LYS73	HD3	1.00	0.013	1.00	15.02
LYS73	HE2	1.00	0.005	1.00	641.65
LYS73	HE3	1.00	0.010	1.00	641.65
LYS73	HA	0.77	0.022	1.00	0.47

3.73.6 Detailed Probabilities of LYS73N:

Overall probability: 0.923

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
SER72	0.67	0.75
LYS73	1.00	1.00
LEU74	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S72H	1.00
S72HG	0.97
S72HB2	1.00
S72HA	1.00
K73HA	1.00
K73HB2	1.00
K73HB3	1.00
K73HG2	1.00
K73HG3	1.00
K73H	1.00
L74H	1.00

NOESY contacts detailed probability

3.73 LYS(73)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER72	HA	1.00	0.060	0.00	0.00
SER72	HB2	1.00	0.008	1.00	-457591.00
SER72	H	1.00	0.005	1.00	-549382.00
LYS73	HA	1.00	0.014	1.00	-830971.00
LYS73	HB2	1.00	0.014	1.00	-1133081.00
LYS73	HB3	1.00	0.013	1.00	-1133081.00
LYS73	HG2	1.00	0.006	1.00	-634765.00
LYS73	HG3	1.00	0.009	1.00	-472196.00
LYS73	H	1.00	0.002	1.00	-6784282.00
LYS73	HD2	0.88	0.009	1.00	-380110.00
LYS73	HD3	0.87	0.008	1.00	-380110.00
LEU74	H	1.00	0.004	1.00	-810082.00
LEU74	HB2	0.61	0.021	1.00	-472196.00

3.73.7 Detailed Probabilities of LYS73HA:

Overall probability: 0.769

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
SER72	0.00	1.00
LYS73	1.00	1.00
LEU74	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S72HA	1.00
K73HB2	1.00
K73HB3	1.00
K73HG2	1.00
K73HG3	1.00
K73HD2	0.98
K73HD3	0.98
K73H	1.00
K73HA	1.00
L74HA	1.00
L74H	1.00

NOESY contacts detailed probability

3.73 LYS(73)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER72	HA	1.00	0.076	0.00	0.00
LYS73	HA	1.00	0.009	1.00	12.17
LYS73	HB2	1.00	0.015	1.00	1.59
LYS73	HB3	1.00	0.015	1.00	1.59
LYS73	HG2	1.00	0.008	1.00	0.44
LYS73	HG3	1.00	0.024	1.00	0.81
LYS73	HD2	0.98	0.020	1.00	1.05
LYS73	HD3	0.98	0.020	1.00	1.05
LYS73	H	1.00	0.014	1.00	-830971.00
LYS73	HE2	0.77	0.022	1.00	0.47
LYS73	HE3	0.76	0.022	1.00	0.47
LEU74	HA	1.00	0.065	0.00	0.00
LEU74	H	1.00	0.060	0.00	0.00

3.73.8 Detailed Probabilities of LYS73HB2:

Overall probability: 0.782

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS73	0.76	1.00
LEU74	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K73HA	1.00
K73HB3	1.00
K73HG2	1.00
K73HG3	1.00
K73HD2	1.00
K73HD3	1.00
K73HE2	0.98
K73HE3	0.99
K73H	1.00
K73HB2	1.00
L74H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS73	HA	1.00	0.024	1.00	2.01
LYS73	HB2	1.00	0.009	1.00	53.87
LYS73	HB3	1.00	0.009	1.00	53.87
LYS73	HG2	1.00	0.023	1.00	2.64
LYS73	HG3	1.00	0.003	1.00	2.94
LYS73	HD2	1.00	0.037	0.30	0.00
LYS73	HD3	1.00	0.037	0.30	0.00
LYS73	HE2	0.98	0.035	0.50	0.00
LYS73	HE3	0.99	0.035	0.50	0.00
LYS73	H	1.00	0.014	1.00	-1133081.00
LEU74	H	1.00	0.007	1.00	-2784560.00

3.73.9 Detailed Probabilities of LYS73HB3:

Overall probability: 0.745

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS73	0.72	1.00
LEU74	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K73HA	1.00
K73HB2	1.00
K73HG2	1.00
K73HG3	1.00
K73HD2	1.00
K73HD3	1.00
K73HE2	0.99
K73HE3	0.99
K73H	1.00
K73HB3	1.00
L74H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS73	HA	1.00	0.025	1.00	2.01
LYS73	HB2	1.00	0.010	1.00	53.87
LYS73	HB3	1.00	0.010	1.00	53.87
LYS73	HG2	1.00	0.024	1.00	2.64
LYS73	HG3	1.00	0.002	1.00	2.94
LYS73	HD2	1.00	0.038	0.20	0.00
LYS73	HD3	1.00	0.038	0.20	0.00
LYS73	HE2	0.99	0.036	0.40	0.00
LYS73	HE3	0.99	0.036	0.40	0.00
LYS73	H	1.00	0.013	1.00	-1133081.00
LEU74	H	1.00	0.008	1.00	-2784560.00

3.73.10 Detailed Probabilities of LYS73HG2:

Overall probability: 0.730

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS73	0.80	0.91
LEU74	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
K73HA	1.00
K73HB2	1.00
K73HB3	1.00
K73HG3	1.00
K73HD2	1.00
K73HD3	1.00
K73HE2	1.00
K73HE3	1.00
K73H	1.00
K73HZ2	1.00
K73HG2	1.00
L74H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS73	HA	1.00	0.017	1.00	0.46
LYS73	HB2	1.00	0.014	1.00	3.20
LYS73	HB3	1.00	0.014	1.00	3.20
LYS73	HG2	1.00	0.003	1.00	27.11
LYS73	HG3	1.00	0.007	1.00	6.42
LYS73	HD2	1.00	0.087	0.00	0.00
LYS73	HD3	1.00	0.087	0.00	0.00
LYS73	HE2	1.00	0.010	1.00	2.64
LYS73	HE3	1.00	0.010	1.00	2.64
LYS73	H	1.00	0.006	1.00	-634765.00
LEU74	H	0.97	0.044	0.03	0.00

3.73.11 Detailed Probabilities of LYS73HG3:

Overall probability: 1.000

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS73	1.00	0.91

Expected NOESY Contacts

Proton	Expected probability
K73HA	1.00
K73HB2	1.00
K73HB3	1.00
K73HG2	1.00
K73HD2	1.00
K73HD3	1.00
K73HE2	1.00
K73HE3	1.00
K73H	1.00
K73HZ2	1.00
K73HG3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS73	HA	1.00	0.010	1.00	0.74
LYS73	HB2	1.00	0.005	1.00	3.41
LYS73	HB3	1.00	0.005	1.00	3.41
LYS73	HG2	1.00	0.019	1.00	7.46
LYS73	HG3	1.00	0.009	1.00	52.13
LYS73	HD2	1.00	0.019	1.00	11.42
LYS73	HD3	1.00	0.019	1.00	11.42
LYS73	HE2	1.00	0.014	1.00	3.64
LYS73	HE3	1.00	0.014	1.00	3.64
LYS73	H	1.00	0.009	1.00	-472196.00

3.73.12 Detailed Probabilities of LYS73HD2:

Overall probability: 0.900

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS73	0.90	0.90

Expected NOESY Contacts

Proton	Expected probability
K73HA	0.98
K73HB2	1.00
K73HB3	1.00
K73HG2	1.00
K73HG3	1.00
K73HD3	1.00
K73HE2	1.00
K73HE3	1.00
K73HZ2	1.00
K73HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS73	HA	0.98	0.003	1.00	0.52
LYS73	HB2	1.00	0.000	1.00	5.56
LYS73	HB3	1.00	0.000	1.00	5.56
LYS73	HG2	1.00	0.059	0.00	0.00
LYS73	HG3	1.00	0.001	1.00	6.34
LYS73	HD2	1.00	0.001	1.00	244.35
LYS73	HD3	1.00	0.001	1.00	244.35
LYS73	HE2	1.00	0.013	1.00	15.02
LYS73	HE3	1.00	0.013	1.00	15.02
LYS73	H	0.87	0.008	1.00	-380110.00

3.73.13 Detailed Probabilities of LYS73HD3:

Overall probability: 0.900

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS73	0.90	0.90

Expected NOESY Contacts

Proton	Expected probability
K73HA	0.98
K73HB2	1.00
K73HB3	1.00
K73HG2	1.00
K73HG3	1.00
K73HD2	1.00
K73HE2	1.00
K73HE3	1.00
K73HZ2	1.00
K73HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS73	HA	0.98	0.003	1.00	0.52
LYS73	HB2	1.00	0.000	1.00	5.56
LYS73	HB3	1.00	0.000	1.00	5.56
LYS73	HG2	1.00	0.059	0.00	0.00
LYS73	HG3	1.00	0.001	1.00	6.34
LYS73	HD2	1.00	0.001	1.00	244.35
LYS73	HD3	1.00	0.001	1.00	244.35
LYS73	HE2	1.00	0.013	1.00	15.02
LYS73	HE3	1.00	0.013	1.00	15.02
LYS73	H	0.87	0.008	1.00	-380110.00

3.73.14 Detailed Probabilities of LYS73HE2:

Overall probability: 0.781

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS73	0.78	0.89

Expected NOESY Contacts

Proton	Expected probability
K73HB2	0.98
K73HB3	0.99
K73HG2	1.00
K73HG3	1.00
K73HD2	1.00
K73HD3	1.00
K73HE3	1.00
K73HZ2	1.00
K73HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS73	HB2	0.98	0.053	0.02	0.00
LYS73	HB3	0.99	0.053	0.01	0.00
LYS73	HG2	1.00	0.011	1.00	0.89
LYS73	HG3	1.00	0.022	1.00	0.86
LYS73	HD2	1.00	0.000	1.00	6.07
LYS73	HD3	1.00	0.000	1.00	6.07
LYS73	HE2	1.00	0.005	1.00	641.65
LYS73	HE3	1.00	0.005	1.00	641.65
LYS73	HA	0.77	0.009	1.00	0.06

3.73.15 Detailed Probabilities of LYS73HE3:

Overall probability: 0.780

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS73	0.78	0.89

Expected NOESY Contacts

Proton	Expected probability
K73HB2	0.99
K73HB3	0.99
K73HG2	1.00
K73HG3	1.00
K73HD2	1.00
K73HD3	1.00
K73HE2	1.00
K73HZ2	1.00
K73HE3	1.00

NOESY contacts detailed probability

3.73 LYS(73)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS73	HB2	0.99	0.048	0.01	0.00
LYS73	HB3	0.99	0.048	0.01	0.00
LYS73	HG2	1.00	0.006	1.00	0.89
LYS73	HG3	1.00	0.017	1.00	0.86
LYS73	HD2	1.00	0.005	1.00	6.07
LYS73	HD3	1.00	0.005	1.00	6.07
LYS73	HE2	1.00	0.010	1.00	641.65
LYS73	HE3	1.00	0.010	1.00	641.65
LYS73	HA	0.76	0.014	1.00	0.06

3.73.16 Detailed Probabilities of LYS73H:

Overall probability: 0.954

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
SER72	1.00	0.75
LYS73	0.92	1.00
LEU74	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S72H	1.00
S72HG	0.97
S72HB2	1.00
S72HA	1.00
K73HA	1.00
K73HB2	1.00
K73HB3	1.00
K73HG2	1.00
K73HG3	1.00
K73H	1.00
L74H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER72	HA	1.00	0.003	1.00	0.20
SER72	HB2	1.00	0.007	1.00	0.21
SER72	H	1.00	0.001	1.00	-644280.00
LYS73	HA	1.00	0.001	1.00	0.66
LYS73	HB2	1.00	0.032	0.80	0.00
LYS73	HB3	1.00	0.032	0.80	0.00
LYS73	HG2	1.00	0.009	1.00	0.38
LYS73	HG3	1.00	0.032	0.80	0.00
LYS73	H	1.00	0.002	1.00	-6784282.00
LYS73	HD2	0.88	0.002	1.00	0.35
LYS73	HD3	0.87	0.002	1.00	0.35
LEU74	H	1.00	0.006	1.00	-824165.00
LEU74	HA	0.91	0.004	1.00	0.08

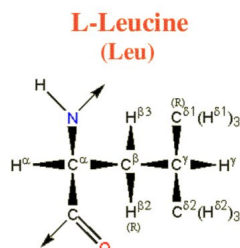
3.74 LEU(74)

Figure 73: Image from the BMRB

Residue probability: 0.650

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	177.332	177.056	1.929	0.000	0.000
CA 3.74.1	55.199	55.735	3.802	0.501	1.000
CB 3.74.2	41.486	42.389	3.750	0.875	1.000
CG 3.74.3	26.267	26.892	3.086	0.629	1.000
CD1 3.74.4	25.818	24.837	3.657	0.333	1.000
CD2 3.74.5	21.875	24.201	3.117	0.833	1.000
N 3.74.6	117.572	121.785	4.943	0.814	1.000
HA 3.74.7	4.227	4.315	0.840	0.645	1.000
HB2 3.74.8	1.466	1.601	0.373	0.513	1.000
HB3 3.74.9	1.197	1.508	0.398	0.875	1.000
HG 3.74.10	1.703	1.510	0.340	0.375	1.000
HD1 3.74.11	0.817	0.739	0.294	0.572	1.000
HD2 3.74.12	0.819	0.727	0.421	0.573	1.000
H 3.74.13	7.609	8.237	0.647	0.907	1.000

3.74.1 Detailed Probabilities of LEU74CA:

Overall probability: 0.501

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS73	0.50	1.00
LEU74	0.43	1.00
GLY75	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
K73HA	1.00
L74HB2	1.00
L74HB3	1.00
L74HG	1.00
L74HD11	0.99
L74HD21	0.99
L74H	1.00
L74HA	1.00
G75HA3	1.00
G75HA2	1.00
G75H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS73	HA	1.00	0.065	0.00	0.00
LYS73	H	0.91	0.004	1.00	0.08
LEU74	HA	1.00	0.001	1.00	6.75
LEU74	HB2	1.00	0.027	1.00	0.32
LEU74	HB3	1.00	0.003	1.00	0.41
LEU74	HG	1.00	0.210	0.00	0.00
LEU74	HD11	0.99	0.095	0.01	0.00
LEU74	HD21	0.99	0.097	0.01	0.00
LEU74	H	1.00	0.110	0.00	0.00
GLY75	HA2	1.00	0.005	1.00	0.07
GLY75	HA3	1.00	0.000	1.00	0.05
GLY75	H	1.00	0.206	0.00	0.00

3.74.2 Detailed Probabilities of LEU74CB:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU74	1.00	1.00
GLY75	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L74HA	1.00
L74HB2	1.00
L74HG	1.00
L74HD11	1.00
L74HD21	1.00
L74H	1.00
L74HB3	1.00
G75H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU74	HA	1.00	0.002	1.00	0.12
LEU74	HB2	1.00	0.014	1.00	0.22
LEU74	HB3	1.00	0.003	1.00	0.32
LEU74	HG	1.00	0.007	1.00	0.09
LEU74	HD11	1.00	0.010	1.00	0.34
LEU74	HD21	1.00	0.008	1.00	0.34
LEU74	H	1.00	0.005	1.00	0.07
GLY75	H	1.00	0.311	0.00	0.00

3.74.3 Detailed Probabilities of LEU74CG:

Overall probability: 0.629

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU74	0.71	1.00
GLY75	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
L74HA	1.00
L74HB2	1.00
L74HB3	1.00
L74HD11	1.00
L74HD21	1.00
L74H	1.00
L74HG	1.00
G75H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU74	HA	1.00	0.003	1.00	0.16
LEU74	HB2	1.00	0.275	0.00	0.00
LEU74	HB3	1.00	0.006	1.00	0.12
LEU74	HG	1.00	0.512	0.00	0.00
LEU74	HD11	1.00	0.008	1.00	1.50
LEU74	HD21	1.00	0.006	1.00	1.50
LEU74	H	1.00	0.005	1.00	0.37
GLY75	H	0.97	0.198	0.03	0.00

3.74.4 Detailed Probabilities of LEU74CD1:

Overall probability: 0.333

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU74	0.33	1.00

Expected NOESY Contacts

Proton	Expected probability
L74HA	0.99
L74HB2	1.00
L74HB3	1.00
L74HG	1.00
L74HD12	1.00
L74HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU74	HA	0.99	0.022	1.00	0.39
LEU74	HB2	1.00	0.255	0.00	0.00
LEU74	HB3	1.00	0.014	1.00	0.36
LEU74	HG	1.00	0.481	0.00	0.00
LEU74	HD11	1.00	0.323	0.00	0.00
LEU74	HD21	1.00	0.321	0.00	0.00

3.74.5 Detailed Probabilities of LEU74CD2:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU74	0.83	1.00

Expected NOESY Contacts

Proton	Expected probability
L74HA	0.99
L74HB2	1.00
L74HB3	1.00
L74HG	1.00
L74HD11	1.00
L74HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU74	HA	0.99	0.001	1.00	2.60
LEU74	HB2	1.00	0.084	0.00	0.00
LEU74	HB3	1.00	0.002	1.00	0.63
LEU74	HG	1.00	0.003	1.00	1.65
LEU74	HD11	1.00	0.005	1.00	88.89
LEU74	HD21	1.00	0.007	1.00	88.89

3.74.6 Detailed Probabilities of LEU74N:

Overall probability: 0.814

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS73	0.67	1.00
LEU74	0.86	1.00
GLY75	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K73HB3	1.00
K73HG2	0.97
K73H	1.00
K73HB2	1.00
K73HA	1.00
L74HA	1.00
L74HB2	1.00
L74HB3	1.00
L74HG	1.00
L74H	1.00
G75H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS73	HA	1.00	0.060	0.00	0.00
LYS73	HB2	1.00	0.007	1.00	-2784560.00
LYS73	HB3	1.00	0.008	1.00	-2784560.00
LYS73	HG2	0.97	0.044	0.03	0.00
LYS73	H	1.00	0.006	1.00	-824165.00
LYS73	HG3	0.95	0.011	1.00	-718382.00
LEU74	HA	1.00	0.004	1.00	-762129.00
LEU74	HB2	1.00	0.023	1.00	-718382.00
LEU74	HB3	1.00	0.003	1.00	-396699.00
LEU74	HG	1.00	0.062	0.00	0.00
LEU74	H	1.00	0.001	1.00	-17911656.00
LEU74	HD11	0.88	0.013	1.00	-1748549.00
LEU74	HD21	0.87	0.011	1.00	-1748549.00
GLY75	H	1.00	0.004	1.00	-717834.00
GLY75	HA2	0.85	0.001	1.00	-950003.00
GLY75	HA3	0.79	0.008	1.00	-495322.00

3.74.7 Detailed Probabilities of LEU74HA:

Overall probability: 0.645

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS73	0.00	1.00
LEU74	0.87	1.00
GLY75	0.33	1.00

Expected NOESY Contacts

Proton	Expected probability
K73HA	1.00
L74HB2	1.00
L74HB3	1.00
L74HG	1.00
L74HD11	0.99
L74HD21	0.99
L74H	1.00
L74HA	1.00
G75HA3	1.00
G75HA2	1.00
G75H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS73	HA	1.00	0.055	0.00	0.00
LEU74	HA	1.00	0.001	1.00	6.75
LEU74	HB2	1.00	0.039	0.10	0.00
LEU74	HB3	1.00	0.002	1.00	0.12
LEU74	HG	1.00	0.003	1.00	0.16
LEU74	HD11	0.99	0.022	1.00	0.39
LEU74	HD21	0.99	0.001	1.00	2.60
LEU74	H	1.00	0.004	1.00	-762129.00
GLY75	HA2	1.00	0.044	0.00	0.00
GLY75	HA3	1.00	0.052	0.00	0.00
GLY75	H	1.00	0.003	1.00	-450553.00

3.74.8 Detailed Probabilities of LEU74HB2:

Overall probability: 0.513

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU74	0.44	1.00
GLY75	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L74HA	1.00
L74HB3	1.00
L74HG	1.00
L74HD11	1.00
L74HD21	1.00
L74H	1.00
L74HB2	1.00
G75H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU74	HA	1.00	0.027	1.00	0.32
LEU74	HB2	1.00	0.039	0.10	0.00
LEU74	HB3	1.00	0.014	1.00	0.22
LEU74	HG	1.00	0.275	0.00	0.00
LEU74	HD11	1.00	0.255	0.00	0.00
LEU74	HD21	1.00	0.084	0.00	0.00
LEU74	H	1.00	0.023	1.00	-718382.00
GLY75	H	1.00	0.027	1.00	-98331.00

3.74.9 Detailed Probabilities of LEU74HB3:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU74	1.00	1.00
GLY75	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L74HA	1.00
L74HB2	1.00
L74HG	1.00
L74HD11	1.00
L74HD21	1.00
L74H	1.00
L74HB3	1.00
G75H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU74	HA	1.00	0.003	1.00	0.41
LEU74	HB2	1.00	0.001	1.00	0.26
LEU74	HB3	1.00	0.003	1.00	0.32
LEU74	HG	1.00	0.006	1.00	0.12
LEU74	HD11	1.00	0.014	1.00	0.36
LEU74	HD21	1.00	0.002	1.00	0.63
LEU74	H	1.00	0.003	1.00	-396699.00
GLY75	H	1.00	0.296	0.00	0.00

3.74.10 Detailed Probabilities of LEU74HG:

Overall probability: 0.375

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU74	0.29	1.00
GLY75	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L74HA	1.00
L74HB2	1.00
L74HB3	1.00
L74HD11	1.00
L74HD21	1.00
L74H	1.00
L74HG	1.00
G75H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU74	HA	1.00	0.210	0.00	0.00
LEU74	HB2	1.00	0.043	0.00	0.00
LEU74	HB3	1.00	0.007	1.00	0.09
LEU74	HG	1.00	0.512	0.00	0.00
LEU74	HD11	1.00	0.481	0.00	0.00
LEU74	HD21	1.00	0.003	1.00	1.65
LEU74	H	1.00	0.062	0.00	0.00
GLY75	H	0.97	0.002	1.00	-100363.00

3.74.11 Detailed Probabilities of LEU74HD11:

Overall probability: 0.572

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU74	0.57	1.00

Expected NOESY Contacts

Proton	Expected probability
L74HA	0.99
L74HB2	1.00
L74HB3	1.00
L74HG	1.00
L74HD12	1.00
L74HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU74	HA	0.99	0.095	0.01	0.00
LEU74	HB2	1.00	0.068	0.00	0.00
LEU74	HB3	1.00	0.010	1.00	0.34
LEU74	HG	1.00	0.008	1.00	1.50
LEU74	HD11	1.00	0.323	0.00	0.00
LEU74	HD21	1.00	0.005	1.00	88.89
LEU74	H	0.86	0.013	1.00	-1748549.00

3.74.12 Detailed Probabilities of LEU74HD21:

Overall probability: 0.573

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU74	0.57	1.00

Expected NOESY Contacts

Proton	Expected probability
L74HA	0.99
L74HB2	1.00
L74HB3	1.00
L74HG	1.00
L74HD11	1.00
L74HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU74	HA	0.99	0.097	0.01	0.00
LEU74	HB2	1.00	0.070	0.00	0.00
LEU74	HB3	1.00	0.008	1.00	0.34
LEU74	HG	1.00	0.006	1.00	1.50
LEU74	HD11	1.00	0.321	0.00	0.00
LEU74	HD21	1.00	0.007	1.00	88.89
LEU74	H	0.85	0.011	1.00	-1748549.00

3.74.13 Detailed Probabilities of LEU74H:

Overall probability: 0.907

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS73	1.00	1.00
LEU74	0.74	1.00
GLY75	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K73HB3	1.00
K73HG2	0.97
K73H	1.00
K73HB2	1.00
K73HA	1.00
L74HA	1.00
L74HB2	1.00
L74HB3	1.00
L74HG	1.00
L74H	1.00
G75H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS73	HA	1.00	0.006	1.00	0.38
LYS73	HB2	1.00	0.006	1.00	2.14
LYS73	HB3	1.00	0.006	1.00	2.14
LYS73	HG2	0.97	0.011	1.00	0.53
LYS73	H	1.00	0.004	1.00	-810082.00
LYS73	HG3	0.95	0.016	1.00	0.15
LEU74	HA	1.00	0.110	0.00	0.00
LEU74	HB2	1.00	0.033	0.70	0.00
LEU74	HB3	1.00	0.005	1.00	0.07
LEU74	HG	1.00	0.005	1.00	0.37
LEU74	H	1.00	0.001	1.00	-17911656.00
GLY75	H	1.00	0.004	1.00	-1129537.00
GLY75	HA2	0.85	0.004	1.00	0.09
GLY75	HA3	0.79	0.012	1.00	0.07

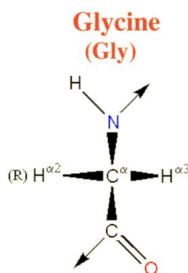
3.75 GLY(75)

Figure 74: 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	174.771	173.872	2.493	0.000	0.000
CA 3.75.1	45.842	45.581	4.381	0.857	1.000
N 3.75.2	105.991	109.752	5.331	0.917	1.000
HA2 3.75.3	3.836	3.967	0.380	1.000	1.000
HA3 3.75.4	4.012	3.897	0.390	0.857	1.000
H 3.75.5	7.925	8.343	0.939	0.730	1.000

3.75.1 Detailed Probabilities of GLY75CA:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU74	0.50	1.00
GLY75	1.00	1.00
TYR76	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L74HA	1.00
G75HA2	1.00
G75H	1.00
G75HA3	1.00
Y76HA	1.00
Y76H	1.00

NOESY contacts detailed probability

3.75 GLY(75)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU74	HA	1.00	0.052	0.00	0.00
LEU74	H	0.79	0.012	1.00	0.07
GLY75	HA2	1.00	0.000	1.00	2.15
GLY75	HA3	1.00	0.004	1.00	4.22
GLY75	H	1.00	0.004	1.00	0.72
TYR76	HA	1.00	0.021	1.00	0.08
TYR76	H	1.00	0.001	1.00	0.16

3.75.2 Detailed Probabilities of GLY75N:

Overall probability: 0.917

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU74	0.86	1.00
GLY75	1.00	1.00
TYR76	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L74HG	0.97
L74H	1.00
L74HA	1.00
L74HB3	1.00
L74HB2	1.00
G75HA2	1.00
G75HA3	1.00
G75H	1.00
Y76H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU74	HA	1.00	0.003	1.00	-450553.00
LEU74	HB2	1.00	0.027	1.00	-98331.00
LEU74	HB3	1.00	0.296	0.00	0.00
LEU74	HG	0.97	0.002	1.00	-100363.00
LEU74	H	1.00	0.004	1.00	-1129537.00
LEU74	HD11	0.51	0.002	1.00	-248364.00
LEU74	HD21	0.53	0.000	1.00	-248364.00
GLY75	HA2	1.00	0.002	1.00	-1025580.00
GLY75	HA3	1.00	0.000	1.00	-1318539.00
GLY75	H	1.00	0.010	1.00	-6976674.00
TYR76	H	1.00	0.000	1.00	-657188.00
TYR76	HA	0.93	0.022	1.00	-510673.00

3.75.3 Detailed Probabilities of GLY75HA2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU74	1.00	1.00
GLY75	1.00	1.00
TYR76	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L74HA	1.00
G75HA3	1.00
G75H	1.00
G75HA2	1.00
Y76HA	1.00
Y76H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU74	HA	1.00	0.005	1.00	0.07
LEU74	H	0.85	0.001	1.00	-950003.00
GLY75	HA2	1.00	0.010	1.00	4.21
GLY75	HA3	1.00	0.000	1.00	2.15
GLY75	H	1.00	0.002	1.00	-1025580.00
TYR76	HA	1.00	0.011	1.00	0.32
TYR76	H	1.00	0.000	1.00	-240757.00

3.75.4 Detailed Probabilities of GLY75HA3:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU74	1.00	1.00
GLY75	1.00	1.00
TYR76	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
L74HA	1.00
G75HA2	1.00
G75H	1.00
G75HA3	1.00
Y76HA	1.00
Y76H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU74	HA	1.00	0.000	1.00	0.05
LEU74	H	0.79	0.008	1.00	-495322.00
GLY75	HA2	1.00	0.003	1.00	2.19
GLY75	HA3	1.00	0.004	1.00	4.22
GLY75	H	1.00	0.000	1.00	-1318539.00
TYR76	HA	1.00	0.165	0.00	0.00
TYR76	H	1.00	0.001	1.00	-229590.00

3.75.5 Detailed Probabilities of GLY75H:

Overall probability: 0.730

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU74	0.58	1.00
GLY75	1.00	1.00
TYR76	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L74HG	0.97
L74H	1.00
L74HA	1.00
L74HB3	1.00
L74HB2	1.00
G75HA2	1.00
G75HA3	1.00
G75H	1.00
Y76H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU74	HA	1.00	0.206	0.00	0.00
LEU74	HB2	1.00	0.013	1.00	0.07
LEU74	HB3	1.00	0.311	0.00	0.00
LEU74	HG	0.97	0.198	0.03	0.00
LEU74	H	1.00	0.004	1.00	-717834.00
LEU74	HD11	0.51	0.004	1.00	0.05
LEU74	HD21	0.53	0.003	1.00	0.06
GLY75	HA2	1.00	0.007	1.00	0.72
GLY75	HA3	1.00	0.004	1.00	0.72
GLY75	H	1.00	0.010	1.00	-6976674.00
TYR76	H	1.00	0.002	1.00	-607258.00

L-Tyrosine (Tyr)

The diagram shows the chemical structure of L-Tyrosine. It features a central alpha-carbon (C^α) bonded to a hydrogen atom (H^α), an amino group (NH₂), a carboxylate group (COO⁻), and a side chain. The side chain consists of a methylene group (CH₂) attached to a para-substituted benzene ring. The benzene ring has protons labeled H^{δ1}, H^{δ2}, H^{δ3}, and H^{δ4}. The side chain is labeled with H^β and C^β. The carboxylate group is labeled with C^γ and O^γ.

Residue probability: 0.813
Residue probability confidence: 1.000

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	175.234	175.405	2.122	0.000	0.000
CA 3.76.1	55.504	58.279	6.333	0.455	1.000
CB 3.76.2	37.962	39.527	6.280	0.667	1.000
CD1 3.76.3	132.040	132.994	20.285	1.000	1.000
CD2 3.76.4	132.146	133.192	23.179	1.000	1.000
CE1 3.76.5	118.075	117.867	2.496	1.000	1.000
CE2 3.76.6	117.910	117.793	3.050	0.667	1.000
N 3.76.7	118.452	120.136	8.494	1.000	1.000
HA 3.76.8	4.778	4.610	0.592	0.917	1.000
HB2 3.76.9	2.664	2.886	0.452	0.667	1.000
HB3 3.76.10	2.848	2.808	0.478	0.625	1.000
HD1 3.76.11	6.856	6.912	0.327	0.813	1.000
HD2 3.76.12	6.856	6.905	0.356	0.813	1.000
HE1 3.76.13	6.715	6.692	0.243	1.000	1.000
HE2 3.76.14	6.715	6.690	0.252	0.667	1.000
H 3.76.15	7.366	8.326	0.740	0.900	1.000
HH	NA	—	—	0.000	0.000

Overall probability: 0.455
Overall confidence: 1.000

Residue	Probability	Confidence
GLY75	0.50	1.00
TYR76	0.43	1.00
LYS77	0.50	1.00

Table of Content

Proton	Expected probability
G75HA2	1.00
G75HA3	1.00
Y76HB2	1.00
Y76HB3	1.00
Y76HD1	1.00
Y76HD2	1.00
Y76H	1.00
Y76HA	1.00
K77H	1.00
K77HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLY75	HA2	1.00	0.011	1.00	0.32
GLY75	HA3	1.00	0.165	0.00	0.00
TYR76	HA	1.00	0.012	1.00	0.37
TYR76	HB2	1.00	0.069	0.00	0.00
TYR76	HB3	1.00	0.115	0.00	0.00
TYR76	HD1	1.00	0.035	0.50	0.00
TYR76	HD2	1.00	0.035	0.50	0.00
TYR76	H	1.00	0.178	0.00	0.00
TYR76	HE1	0.75	0.024	1.00	0.38
LYS77	HA	1.00	0.218	0.00	0.00
LYS77	H	1.00	0.012	1.00	0.31

3.76.2 Detailed Probabilities of TYR76CB:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR76	0.71	1.00
LYS77	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
Y76HA	1.00
Y76HB2	1.00
Y76HD1	1.00
Y76HD2	1.00
Y76HE2	1.00
Y76H	1.00
Y76HB3	1.00
K77H	1.00

NOESY contacts detailed probability

3.76 TYR(76)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR76	HA	1.00	0.012	1.00	0.21
TYR76	HB2	1.00	0.006	1.00	0.59
TYR76	HB3	1.00	0.178	0.00	0.00
TYR76	HD1	1.00	0.001	1.00	0.25
TYR76	HD2	1.00	0.001	1.00	0.25
TYR76	HE2	1.00	0.140	0.00	0.00
TYR76	H	1.00	0.001	1.00	0.09
LYS77	H	1.00	0.051	0.00	0.00
LYS77	HA	0.84	0.020	1.00	1.14

3.76.3 Detailed Probabilities of TYR76CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR76	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y76HA	1.00
Y76HB2	1.00
Y76HB3	1.00
Y76HD2	1.00
Y76HE1	1.00
Y76HE2	1.00
Y76H	1.00
Y76HD1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR76	HA	1.00	0.012	1.00	0.83
TYR76	HB2	1.00	0.001	1.00	0.63
TYR76	HB3	1.00	0.012	1.00	0.60
TYR76	HD1	1.00	0.003	1.00	9.22
TYR76	HD2	1.00	0.003	1.00	9.22
TYR76	HE1	1.00	0.011	1.00	2.42
TYR76	HE2	1.00	0.011	1.00	2.42
TYR76	H	1.00	0.001	1.00	0.50

3.76.4 Detailed Probabilities of TYR76CD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR76	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y76HA	1.00
Y76HB2	1.00
Y76HB3	1.00
Y76HD1	1.00
Y76HE1	1.00
Y76HE2	1.00
Y76H	0.98
Y76HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR76	HA	1.00	0.012	1.00	0.83
TYR76	HB2	1.00	0.001	1.00	0.63
TYR76	HB3	1.00	0.012	1.00	0.60
TYR76	HD1	1.00	0.003	1.00	9.22
TYR76	HD2	1.00	0.003	1.00	9.22
TYR76	HE1	1.00	0.011	1.00	2.42
TYR76	HE2	1.00	0.011	1.00	2.42
TYR76	H	0.98	0.001	1.00	0.50

3.76.5 Detailed Probabilities of TYR76CE1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR76	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y76HD1	1.00
Y76HD2	1.00
Y76HE2	1.00
Y76HE1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR76	HD1	1.00	0.006	1.00	2.80
TYR76	HD2	1.00	0.006	1.00	2.80
TYR76	HE1	1.00	0.005	1.00	34.17
TYR76	HE2	1.00	0.005	1.00	34.17
TYR76	HA	0.75	0.026	1.00	1.31

3.76.6 Detailed Probabilities of TYR76CE2:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR76	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
Y76HB2	1.00
Y76HB3	1.00
Y76HD1	1.00
Y76HD2	1.00
Y76HE1	1.00
Y76HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR76	HB2	1.00	0.085	0.00	0.00
TYR76	HB3	1.00	0.056	0.00	0.00
TYR76	HD1	1.00	0.006	1.00	2.80
TYR76	HD2	1.00	0.006	1.00	2.80
TYR76	HE1	1.00	0.005	1.00	34.17
TYR76	HE2	1.00	0.005	1.00	34.17

3.76.7 Detailed Probabilities of TYR76N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLY75	1.00	1.00
TYR76	1.00	1.00
LYS77	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
G75HA2	1.00
G75HA3	1.00
G75H	1.00
Y76HA	1.00
Y76HB2	1.00
Y76HB3	1.00
Y76HD1	1.00
Y76HD2	0.98
Y76H	1.00
K77H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLY75	HA2	1.00	0.000	1.00	-240757.00
GLY75	HA3	1.00	0.001	1.00	-229590.00
GLY75	H	1.00	0.002	1.00	-607258.00
TYR76	HA	1.00	0.001	1.00	-309060.00
TYR76	HB2	1.00	0.002	1.00	-616974.00
TYR76	HB3	1.00	0.007	1.00	-339459.00
TYR76	HD1	1.00	0.002	1.00	-595370.00
TYR76	HD2	0.98	0.002	1.00	-595370.00
TYR76	H	1.00	0.000	1.00	-6617762.00
LYS77	H	1.00	0.009	1.00	-114622.00

3.76.8 Detailed Probabilities of TYR76HA:

Overall probability: 0.917

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLY75	1.00	1.00
TYR76	1.00	1.00
LYS77	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
G75HA2	1.00
G75HA3	1.00
Y76HB2	1.00
Y76HB3	1.00
Y76HD1	1.00
Y76HD2	1.00
Y76H	1.00
Y76HA	1.00
K77H	1.00
K77HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLY75	HA2	1.00	0.004	1.00	0.10
GLY75	HA3	1.00	0.021	1.00	0.08
GLY75	H	0.93	0.022	1.00	-510673.00
TYR76	HA	1.00	0.012	1.00	0.37
TYR76	HB2	1.00	0.003	1.00	0.13
TYR76	HB3	1.00	0.012	1.00	0.21
TYR76	HD1	1.00	0.012	1.00	0.83
TYR76	HD2	1.00	0.012	1.00	0.83
TYR76	H	1.00	0.001	1.00	-309060.00
TYR76	HE1	0.75	0.026	1.00	1.31
LYS77	HA	1.00	0.524	0.00	0.00
LYS77	H	1.00	0.011	1.00	-631564.00

3.76.9 Detailed Probabilities of TYR76HB2:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR76	0.57	1.00
LYS77	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y76HA	1.00
Y76HB3	1.00
Y76HD1	1.00
Y76HD2	1.00
Y76HE2	1.00
Y76H	1.00
Y76HB2	1.00
K77H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR76	HA	1.00	0.069	0.00	0.00
TYR76	HB2	1.00	0.185	0.00	0.00
TYR76	HB3	1.00	0.006	1.00	0.59
TYR76	HD1	1.00	0.001	1.00	0.63
TYR76	HD2	1.00	0.001	1.00	0.63
TYR76	HE2	1.00	0.085	0.00	0.00
TYR76	H	1.00	0.002	1.00	-616974.00
LYS77	H	1.00	0.004	1.00	-281448.00
LYS77	HA	0.61	0.023	1.00	0.14

3.76.10 Detailed Probabilities of TYR76HB3:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR76	0.57	1.00
LYS77	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y76HA	1.00
Y76HB2	1.00
Y76HD1	1.00
Y76HD2	1.00
Y76HE2	1.00
Y76H	1.00
Y76HB3	1.00
K77H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR76	HA	1.00	0.115	0.00	0.00
TYR76	HB2	1.00	0.001	1.00	0.69
TYR76	HB3	1.00	0.178	0.00	0.00
TYR76	HD1	1.00	0.012	1.00	0.60
TYR76	HD2	1.00	0.012	1.00	0.60
TYR76	HE2	1.00	0.056	0.00	0.00
TYR76	H	1.00	0.007	1.00	-339459.00
LYS77	H	1.00	0.005	1.00	-403143.00

3.76.11 Detailed Probabilities of TYR76HD1:

Overall probability: 0.813

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR76	0.81	1.00

Expected NOESY Contacts

Proton	Expected probability
Y76HA	1.00
Y76HB2	1.00
Y76HB3	1.00
Y76HD2	1.00
Y76HE1	1.00
Y76HE2	1.00
Y76H	1.00
Y76HD1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR76	HA	1.00	0.035	0.50	0.00
TYR76	HB2	1.00	0.511	0.00	0.00
TYR76	HB3	1.00	0.001	1.00	0.25
TYR76	HD1	1.00	0.003	1.00	9.22
TYR76	HD2	1.00	0.003	1.00	9.22
TYR76	HE1	1.00	0.006	1.00	2.80
TYR76	HE2	1.00	0.006	1.00	2.80
TYR76	H	1.00	0.002	1.00	-595370.00

3.76.12 Detailed Probabilities of TYR76HD2:

Overall probability: 0.813

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR76	0.81	1.00

Expected NOESY Contacts

Proton	Expected probability
Y76HA	1.00
Y76HB2	1.00
Y76HB3	1.00
Y76HD1	1.00
Y76HE1	1.00
Y76HE2	1.00
Y76H	0.98
Y76HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR76	HA	1.00	0.035	0.50	0.00
TYR76	HB2	1.00	0.511	0.00	0.00
TYR76	HB3	1.00	0.001	1.00	0.25
TYR76	HD1	1.00	0.003	1.00	9.22
TYR76	HD2	1.00	0.003	1.00	9.22
TYR76	HE1	1.00	0.006	1.00	2.80
TYR76	HE2	1.00	0.006	1.00	2.80
TYR76	H	0.98	0.002	1.00	-595370.00

3.76.13 Detailed Probabilities of TYR76HE1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR76	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y76HD1	1.00
Y76HD2	1.00
Y76HE2	1.00
Y76HE1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR76	HD1	1.00	0.011	1.00	2.42
TYR76	HD2	1.00	0.011	1.00	2.42
TYR76	HE1	1.00	0.005	1.00	34.17
TYR76	HE2	1.00	0.005	1.00	34.17
TYR76	HA	0.75	0.024	1.00	0.38

3.76.14 Detailed Probabilities of TYR76HE2:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR76	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
Y76HB2	1.00
Y76HB3	1.00
Y76HD1	1.00
Y76HD2	1.00
Y76HE1	1.00
Y76HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR76	HB2	1.00	0.652	0.00	0.00
TYR76	HB3	1.00	0.140	0.00	0.00
TYR76	HD1	1.00	0.011	1.00	2.42
TYR76	HD2	1.00	0.011	1.00	2.42
TYR76	HE1	1.00	0.005	1.00	34.17
TYR76	HE2	1.00	0.005	1.00	34.17

3.76.15 Detailed Probabilities of TYR76H:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLY75	1.00	1.00
TYR76	0.83	1.00
LYS77	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
G75HA2	1.00
G75HA3	1.00
G75H	1.00
Y76HA	1.00
Y76HB2	1.00
Y76HB3	1.00
Y76HD1	1.00
Y76HD2	0.98
Y76H	1.00
K77H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLY75	HA2	1.00	0.005	1.00	0.22
GLY75	HA3	1.00	0.001	1.00	0.16
GLY75	H	1.00	0.000	1.00	-657188.00
TYR76	HA	1.00	0.178	0.00	0.00
TYR76	HB2	1.00	0.001	1.00	0.20
TYR76	HB3	1.00	0.001	1.00	0.09
TYR76	HD1	1.00	0.001	1.00	0.50
TYR76	HD2	0.98	0.001	1.00	0.50
TYR76	H	1.00	0.000	1.00	-6617762.00
LYS77	H	1.00	0.001	1.00	-76987.00

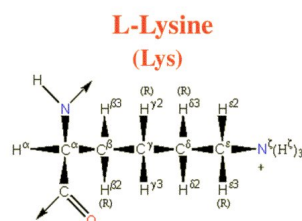


Figure 76: Image from the BMRB

Residue probability: 0.712
Residue probability confidence: 0.945

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.138	176.660	3.133	0.000	0.000
CA 3.77.1	55.070	57.014	3.028	0.769	1.000
CB 3.77.2	32.217	32.981	3.186	0.365	1.000
CG 3.77.3	24.491	24.941	1.956	1.000	0.917
CD 3.77.4	28.205	29.020	2.193	0.700	0.900
CE 3.77.5	41.931	41.893	1.492	0.780	0.889
N 3.77.6	122.866	120.954	4.210	0.923	1.000
NZ	NA	—	—	0.000	0.000
HA 3.77.7	4.548	4.262	0.489	0.820	1.000
HB2 3.77.8	1.843	1.774	0.365	0.639	1.000
HB3 3.77.9	1.841	1.742	0.385	0.638	1.000
HG2 3.77.10	1.355	1.358	0.344	0.636	0.917
HG3 3.77.11	1.171	1.343	0.357	0.818	0.917
HD2 3.77.12	1.624	1.614	0.957	0.444	0.900
HD3 3.77.13	1.623	1.595	0.387	0.444	0.900
HE2 3.77.14	2.825	2.907	0.230	0.750	0.889
HE3 3.77.15	2.576	2.901	0.241	0.753	0.889
H 3.77.16	8.290	8.185	0.605	0.913	1.000
HZ	NA	—	—	0.000	0.000

3.77.1 Detailed Probabilities of LYS77CA:

Overall probability: 0.769
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR76	0.50	1.00
LYS77	0.88	1.00
VAL78	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
Y76HA	1.00
K77HB2	1.00
K77HB3	1.00
K77HG2	1.00
K77HG3	1.00
K77HD2	0.98
K77HD3	0.98
K77H	1.00
K77HA	1.00
V78HA	1.00
V78H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR76	HA	1.00	0.524	0.00	0.00
TYR76	HB2	0.61	0.023	1.00	0.14
LYS77	HA	1.00	0.309	0.00	0.00
LYS77	HB2	1.00	0.002	1.00	0.82
LYS77	HB3	1.00	0.004	1.00	0.82
LYS77	HG2	1.00	0.006	1.00	0.27
LYS77	HG3	1.00	0.003	1.00	0.20
LYS77	HD2	0.98	0.008	1.00	0.58
LYS77	HD3	0.98	0.009	1.00	0.58
LYS77	H	1.00	0.019	1.00	0.30
VAL78	HA	1.00	0.136	0.00	0.00
VAL78	H	1.00	0.006	1.00	1.39
VAL78	HG21	0.50	0.005	1.00	0.13

3.77.2 Detailed Probabilities of LYS77CB:

Overall probability: 0.365

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS77	0.40	1.00
VAL78	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K77HA	1.00
K77HB2	1.00
K77HG2	1.00
K77HG3	1.00
K77HD2	1.00
K77HD3	1.00
K77HE2	0.99
K77HE3	0.99
K77H	1.00
K77HB3	1.00
V78H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS77	HA	1.00	0.001	1.00	0.92
LYS77	HB2	1.00	0.657	0.00	0.00
LYS77	HB3	1.00	0.655	0.00	0.00
LYS77	HG2	1.00	0.169	0.00	0.00
LYS77	HG3	1.00	0.015	1.00	0.52
LYS77	HD2	1.00	0.438	0.00	0.00
LYS77	HD3	1.00	0.437	0.00	0.00
LYS77	HE2	0.99	0.010	1.00	0.05
LYS77	HE3	0.99	0.259	0.01	0.00
LYS77	H	1.00	0.007	1.00	0.39
VAL78	H	1.00	0.467	0.00	0.00

3.77.3 Detailed Probabilities of LYS77CG:

Overall probability: 1.000

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS77	1.00	0.91
VAL78	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K77HA	1.00
K77HB2	1.00
K77HB3	1.00
K77HG2	1.00
K77HD2	1.00
K77HD3	1.00
K77HE2	1.00
K77HE3	1.00
K77H	1.00
K77HZ2	1.00
K77HG3	1.00
V78H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS77	HA	1.00	0.003	1.00	0.20
LYS77	HB2	1.00	0.005	1.00	0.69
LYS77	HB3	1.00	0.007	1.00	0.69
LYS77	HG2	1.00	0.004	1.00	2.48
LYS77	HG3	1.00	0.004	1.00	4.79
LYS77	HD2	1.00	0.002	1.00	0.78
LYS77	HD3	1.00	0.003	1.00	0.78
LYS77	HE2	1.00	0.005	1.00	0.16
LYS77	HE3	1.00	0.004	1.00	0.27
LYS77	H	1.00	0.001	1.00	0.07
VAL78	H	0.96	0.004	1.00	0.16

3.77.4 Detailed Probabilities of LYS77CD:

Overall probability: 0.700

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS77	0.70	0.90

Expected NOESY Contacts

Proton	Expected probability
K77HA	0.98
K77HB2	1.00
K77HB3	1.00
K77HG2	1.00
K77HG3	1.00
K77HD3	1.00
K77HE2	1.00
K77HE3	1.00
K77HZ2	1.00
K77HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS77	HA	0.98	0.000	1.00	0.64
LYS77	HB2	1.00	0.003	1.00	0.49
LYS77	HB3	1.00	0.001	1.00	0.49
LYS77	HG2	1.00	0.007	1.00	0.81
LYS77	HG3	1.00	0.191	0.00	0.00
LYS77	HD2	1.00	0.216	0.00	0.00
LYS77	HD3	1.00	0.217	0.00	0.00
LYS77	HE2	1.00	0.001	1.00	0.62
LYS77	HE3	1.00	0.001	1.00	0.62
LYS77	H	0.88	0.015	1.00	0.06

3.77.5 Detailed Probabilities of LYS77CE:

Overall probability: 0.780

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS77	0.78	0.89

Expected NOESY Contacts

Proton	Expected probability
K77HB2	0.99
K77HB3	0.99
K77HG2	1.00
K77HG3	1.00
K77HD2	1.00
K77HD3	1.00
K77HE2	1.00
K77HZ2	1.00
K77HE3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS77	HB2	0.99	0.213	0.01	0.00
LYS77	HB3	0.99	0.211	0.01	0.00
LYS77	HG2	1.00	0.002	1.00	0.20
LYS77	HG3	1.00	0.004	1.00	0.40
LYS77	HD2	1.00	0.006	1.00	0.99
LYS77	HD3	1.00	0.007	1.00	0.99
LYS77	HE2	1.00	0.004	1.00	4.70
LYS77	HE3	1.00	0.003	1.00	11.95
LYS77	HA	0.76	0.009	1.00	0.07

3.77.6 Detailed Probabilities of LYS77N:

Overall probability: 0.923

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR76	1.00	1.00
LYS77	0.83	1.00
VAL78	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y76H	1.00
Y76HB3	1.00
Y76HA	1.00
Y76HB2	1.00
K77HA	1.00
K77HB2	1.00
K77HB3	1.00
K77HG2	1.00
K77HG3	1.00
K77H	1.00
V78H	1.00

NOESY contacts detailed probability

3.77 LYS(77)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR76	HA	1.00	0.011	1.00	-631564.00
TYR76	HB2	1.00	0.004	1.00	-281448.00
TYR76	HB3	1.00	0.005	1.00	-403143.00
TYR76	H	1.00	0.001	1.00	-76987.00
TYR76	HD1	0.79	0.001	1.00	-207367.00
TYR76	HD2	0.66	0.001	1.00	-207367.00
LYS77	HA	1.00	0.023	1.00	-463801.00
LYS77	HB2	1.00	0.005	1.00	-727474.00
LYS77	HB3	1.00	0.007	1.00	-727474.00
LYS77	HG2	1.00	0.183	0.00	0.00
LYS77	HG3	1.00	0.001	1.00	-86032.00
LYS77	H	1.00	0.014	1.00	-5070981.00
VAL78	H	1.00	0.005	1.00	-100425.00

3.77.7 Detailed Probabilities of LYS77HA:

Overall probability: 0.820

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR76	0.50	1.00
LYS77	0.90	1.00
VAL78	0.77	1.00

Expected NOESY Contacts

Proton	Expected probability
Y76HA	1.00
K77HB2	1.00
K77HB3	1.00
K77HG2	1.00
K77HG3	1.00
K77HD2	0.98
K77HD3	0.98
K77H	1.00
K77HA	1.00
V78HA	1.00
V78H	1.00

NOESY contacts detailed probability

3.77 LYS(77)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR76	HA	1.00	0.218	0.00	0.00
TYR76	HB3	0.84	0.020	1.00	1.14
LYS77	HA	1.00	0.309	0.00	0.00
LYS77	HB2	1.00	0.001	1.00	0.92
LYS77	HB3	1.00	0.001	1.00	0.92
LYS77	HG2	1.00	0.000	1.00	0.10
LYS77	HG3	1.00	0.003	1.00	0.20
LYS77	HD2	0.98	0.000	1.00	0.64
LYS77	HD3	0.98	0.000	1.00	0.64
LYS77	H	1.00	0.023	1.00	-463801.00
LYS77	HE2	0.77	0.025	1.00	0.17
LYS77	HE3	0.76	0.009	1.00	0.07
VAL78	HA	1.00	0.037	0.30	0.00
VAL78	H	1.00	0.000	1.00	-1716215.00
VAL78	HG21	0.50	0.001	1.00	0.21

3.77.8 Detailed Probabilities of LYS77HB2:

Overall probability: 0.639

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS77	0.60	1.00
VAL78	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K77HA	1.00
K77HB3	1.00
K77HG2	1.00
K77HG3	1.00
K77HD2	1.00
K77HD3	1.00
K77HE2	0.98
K77HE3	0.99
K77H	1.00
K77HB2	1.00
V78H	1.00

NOESY contacts detailed probability

3.77 LYS(77)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS77	HA	1.00	0.002	1.00	0.82
LYS77	HB2	1.00	0.657	0.00	0.00
LYS77	HB3	1.00	0.657	0.00	0.00
LYS77	HG2	1.00	0.016	1.00	0.97
LYS77	HG3	1.00	0.005	1.00	0.69
LYS77	HD2	1.00	0.003	1.00	0.49
LYS77	HD3	1.00	0.003	1.00	0.49
LYS77	HE2	0.98	0.082	0.02	0.00
LYS77	HE3	0.99	0.213	0.01	0.00
LYS77	H	1.00	0.005	1.00	-727474.00
VAL78	H	1.00	0.004	1.00	-244516.00

3.77.9 Detailed Probabilities of LYS77HB3:

Overall probability: 0.638

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS77	0.60	1.00
VAL78	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K77HA	1.00
K77HB2	1.00
K77HG2	1.00
K77HG3	1.00
K77HD2	1.00
K77HD3	1.00
K77HE2	0.99
K77HE3	0.99
K77H	1.00
K77HB3	1.00
V78H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS77	HA	1.00	0.004	1.00	0.82
LYS77	HB2	1.00	0.655	0.00	0.00
LYS77	HB3	1.00	0.655	0.00	0.00
LYS77	HG2	1.00	0.018	1.00	0.97
LYS77	HG3	1.00	0.007	1.00	0.69
LYS77	HD2	1.00	0.001	1.00	0.49
LYS77	HD3	1.00	0.001	1.00	0.49
LYS77	HE2	0.99	0.084	0.01	0.00
LYS77	HE3	0.99	0.211	0.01	0.00
LYS77	H	1.00	0.007	1.00	-727474.00
VAL78	H	1.00	0.006	1.00	-244516.00

3.77.10 Detailed Probabilities of LYS77HG2:

Overall probability: 0.636

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS77	0.60	0.91
VAL78	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K77HA	1.00
K77HB2	1.00
K77HB3	1.00
K77HG3	1.00
K77HD2	1.00
K77HD3	1.00
K77HE2	1.00
K77HE3	1.00
K77H	1.00
K77HZ2	1.00
K77HG2	1.00
V78H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS77	HA	1.00	0.006	1.00	0.27
LYS77	HB2	1.00	0.169	0.00	0.00
LYS77	HB3	1.00	0.169	0.00	0.00
LYS77	HG2	1.00	0.029	1.00	36.93
LYS77	HG3	1.00	0.004	1.00	2.48
LYS77	HD2	1.00	0.007	1.00	0.81
LYS77	HD3	1.00	0.007	1.00	0.81
LYS77	HE2	1.00	0.082	0.00	0.00
LYS77	HE3	1.00	0.002	1.00	0.20
LYS77	H	1.00	0.183	0.00	0.00
VAL78	H	0.98	0.002	1.00	-79349.00

3.77.11 Detailed Probabilities of LYS77HG3:

Overall probability: 0.818

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS77	0.80	0.91
VAL78	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K77HA	1.00
K77HB2	1.00
K77HB3	1.00
K77HG2	1.00
K77HD2	1.00
K77HD3	1.00
K77HE2	1.00
K77HE3	1.00
K77H	1.00
K77HZ2	1.00
K77HG3	1.00
V78H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS77	HA	1.00	0.003	1.00	0.20
LYS77	HB2	1.00	0.015	1.00	0.52
LYS77	HB3	1.00	0.015	1.00	0.52
LYS77	HG2	1.00	0.011	1.00	2.41
LYS77	HG3	1.00	0.004	1.00	4.79
LYS77	HD2	1.00	0.191	0.00	0.00
LYS77	HD3	1.00	0.191	0.00	0.00
LYS77	HE2	1.00	0.004	1.00	0.25
LYS77	HE3	1.00	0.004	1.00	0.40
LYS77	H	1.00	0.001	1.00	-86032.00
VAL78	H	0.96	0.001	1.00	-183943.00

3.77.12 Detailed Probabilities of LYS77HD2:

Overall probability: 0.444

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS77	0.44	0.90

Expected NOESY Contacts

Proton	Expected probability
K77HA	0.98
K77HB2	1.00
K77HB3	1.00
K77HG2	1.00
K77HG3	1.00
K77HD3	1.00
K77HE2	1.00
K77HE3	1.00
K77HZ2	1.00
K77HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS77	HA	0.98	0.008	1.00	0.58
LYS77	HB2	1.00	0.438	0.00	0.00
LYS77	HB3	1.00	0.438	0.00	0.00
LYS77	HG2	1.00	0.092	0.00	0.00
LYS77	HG3	1.00	0.002	1.00	0.78
LYS77	HD2	1.00	0.216	0.00	0.00
LYS77	HD3	1.00	0.216	0.00	0.00
LYS77	HE2	1.00	0.025	1.00	2.01
LYS77	HE3	1.00	0.006	1.00	0.99

3.77.13 Detailed Probabilities of LYS77HD3:

Overall probability: 0.444

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS77	0.44	0.90

Expected NOESY Contacts

Proton	Expected probability
K77HA	0.98
K77HB2	1.00
K77HB3	1.00
K77HG2	1.00
K77HG3	1.00
K77HD2	1.00
K77HE2	1.00
K77HE3	1.00
K77HZ2	1.00
K77HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS77	HA	0.98	0.009	1.00	0.58
LYS77	HB2	1.00	0.437	0.00	0.00
LYS77	HB3	1.00	0.437	0.00	0.00
LYS77	HG2	1.00	0.091	0.00	0.00
LYS77	HG3	1.00	0.003	1.00	0.78
LYS77	HD2	1.00	0.217	0.00	0.00
LYS77	HD3	1.00	0.217	0.00	0.00
LYS77	HE2	1.00	0.026	1.00	2.01
LYS77	HE3	1.00	0.007	1.00	0.99

3.77.14 Detailed Probabilities of LYS77HE2:

Overall probability: 0.750

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS77	0.75	0.89

Expected NOESY Contacts

Proton	Expected probability
K77HB2	0.98
K77HB3	0.99
K77HG2	1.00
K77HG3	1.00
K77HD2	1.00
K77HD3	1.00
K77HE3	1.00
K77HZ2	1.00
K77HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS77	HB2	0.98	0.010	1.00	0.05
LYS77	HB3	0.99	0.010	1.00	0.05
LYS77	HG2	1.00	0.043	0.00	0.00
LYS77	HG3	1.00	0.005	1.00	0.16
LYS77	HD2	1.00	0.001	1.00	0.62
LYS77	HD3	1.00	0.001	1.00	0.62
LYS77	HE2	1.00	0.045	0.00	0.00
LYS77	HE3	1.00	0.004	1.00	4.70

3.77.15 Detailed Probabilities of LYS77HE3:

Overall probability: 0.753

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS77	0.75	0.89

Expected NOESY Contacts

Proton	Expected probability
K77HB2	0.99
K77HB3	0.99
K77HG2	1.00
K77HG3	1.00
K77HD2	1.00
K77HD3	1.00
K77HE2	1.00
K77HZ2	1.00
K77HE3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS77	HB2	0.99	0.259	0.01	0.00
LYS77	HB3	0.99	0.259	0.01	0.00
LYS77	HG2	1.00	0.001	1.00	0.14
LYS77	HG3	1.00	0.004	1.00	0.27
LYS77	HD2	1.00	0.001	1.00	0.62
LYS77	HD3	1.00	0.001	1.00	0.62
LYS77	HE2	1.00	0.002	1.00	4.53
LYS77	HE3	1.00	0.003	1.00	11.95

3.77.16 Detailed Probabilities of LYS77H:

Overall probability: 0.913

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR76	0.83	1.00
LYS77	1.00	1.00
VAL78	0.70	1.00

Expected NOESY Contacts

Proton	Expected probability
Y76H	1.00
Y76HB3	1.00
Y76HA	1.00
Y76HB2	1.00
K77HA	1.00
K77HB2	1.00
K77HB3	1.00
K77HG2	1.00
K77HG3	1.00
K77H	1.00
V78H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR76	HA	1.00	0.012	1.00	0.31
TYR76	HB2	1.00	0.015	1.00	0.10
TYR76	HB3	1.00	0.051	0.00	0.00
TYR76	H	1.00	0.009	1.00	-114622.00
TYR76	HD1	0.79	0.013	1.00	0.23
TYR76	HD2	0.66	0.013	1.00	0.23
LYS77	HA	1.00	0.019	1.00	0.30
LYS77	HB2	1.00	0.007	1.00	0.39
LYS77	HB3	1.00	0.007	1.00	0.39
LYS77	HG2	1.00	0.003	1.00	0.11
LYS77	HG3	1.00	0.001	1.00	0.07
LYS77	H	1.00	0.014	1.00	-5070981.00
LYS77	HD2	0.88	0.015	1.00	0.06
LYS77	HD3	0.87	0.015	1.00	0.06
VAL78	H	1.00	0.033	0.70	0.00

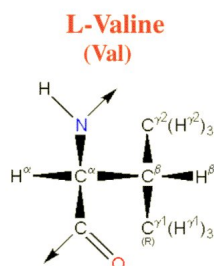
3.78 VAL(78)

Figure 77: Image from the BMRB

Residue probability: 0.861

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.162	175.682	2.367	0.000	0.000
CA 3.78.1	60.229	62.613	4.828	0.922	1.000
CB 3.78.2	34.355	32.918	4.591	1.000	1.000
CG1 3.78.3	21.108	21.563	2.746	0.714	1.000
CG2 3.78.4	22.145	21.368	2.801	0.800	1.000
N 3.78.5	124.071	121.057	5.832	0.900	1.000
HA 3.78.6	5.166	4.178	0.599	0.750	1.000
HB 3.78.7	1.557	1.980	0.322	1.000	1.000
HG1 3.78.8	0.615	0.816	0.264	0.857	1.000
HG2 3.78.9	0.725	0.803	0.504	1.000	1.000
H 3.78.10	7.830	8.311	0.669	0.671	1.000

3.78.1 Detailed Probabilities of VAL78CA:

Overall probability: 0.922

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS77	0.30	1.00
VAL78	1.00	1.00
PHE79	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K77HA	1.00
V78HG11	1.00
V78HG21	1.00
V78H	1.00
V78HB	1.00
V78HA	1.00
F79H	1.00
F79HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS77	HA	1.00	0.037	0.30	0.00
VAL78	HA	1.00	0.001	1.00	2.12
VAL78	HB	1.00	0.000	1.00	0.28
VAL78	HG11	1.00	0.006	1.00	0.54
VAL78	HG21	1.00	0.003	1.00	0.55
VAL78	H	1.00	0.009	1.00	0.16
PHE79	HA	1.00	0.018	1.00	0.06
PHE79	H	1.00	0.005	1.00	1.16
PHE79	HB2	0.52	0.022	1.00	0.10

3.78.2 Detailed Probabilities of VAL78CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL78	1.00	1.00
PHE79	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V78HA	1.00
V78HG11	1.00
V78HG21	1.00
V78H	1.00
V78HB	1.00
F79H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL78	HA	1.00	0.003	1.00	0.21
VAL78	HB	1.00	0.005	1.00	3.52
VAL78	HG11	1.00	0.001	1.00	1.07
VAL78	HG21	1.00	0.003	1.00	1.14
VAL78	H	1.00	0.005	1.00	0.54
PHE79	H	1.00	0.006	1.00	0.10
PHE79	HA	0.85	0.015	1.00	0.17

3.78.3 Detailed Probabilities of VAL78CG1:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL78	0.60	1.00
PHE79	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V78HA	1.00
V78HG12	1.00
V78HG21	1.00
V78H	1.00
V78HB	1.00
F79H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL78	HA	1.00	0.000	1.00	0.70
VAL78	HB	1.00	0.002	1.00	1.60
VAL78	HG11	1.00	0.119	0.00	0.00
VAL78	HG21	1.00	0.009	1.00	4.37
VAL78	H	1.00	0.546	0.00	0.00
PHE79	H	0.98	0.002	1.00	0.63
PHE79	HA	0.60	0.009	1.00	0.22

3.78.4 Detailed Probabilities of VAL78CG2:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL78	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
V78HA	1.00
V78HG11	1.00
V78HG22	1.00
V78H	1.00
V78HB	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL78	HA	1.00	0.619	0.00	0.00
VAL78	HB	1.00	0.003	1.00	1.54
VAL78	HG11	1.00	0.005	1.00	2.76
VAL78	HG21	1.00	0.005	1.00	46.27
VAL78	H	1.00	0.004	1.00	0.71

3.78.5 Detailed Probabilities of VAL78N:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS77	0.95	1.00
VAL78	1.00	1.00
PHE79	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K77HG2	0.98
K77HG3	0.96
K77HA	1.00
K77HB3	1.00
K77HB2	1.00
K77H	1.00
V78HA	1.00
V78HG11	1.00
V78HG21	1.00
V78HB	1.00
V78H	1.00
F79H	1.00
F79HA	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS77	HA	1.00	0.000	1.00	-1716215.00
LYS77	HB2	1.00	0.004	1.00	-244516.00
LYS77	HB3	1.00	0.006	1.00	-244516.00
LYS77	HG2	0.98	0.002	1.00	-79349.00
LYS77	HG3	0.96	0.001	1.00	-183943.00
LYS77	H	1.00	0.033	0.70	0.00
VAL78	HA	1.00	0.006	1.00	-251004.00
VAL78	HB	1.00	0.010	1.00	-670087.00
VAL78	HG11	1.00	0.000	1.00	-354862.00
VAL78	HG21	1.00	0.002	1.00	-648934.00
VAL78	H	1.00	0.004	1.00	-4592120.00
PHE79	HA	0.96	0.019	1.00	-1716215.00
PHE79	H	1.00	0.051	0.00	0.00

3.78.6 Detailed Probabilities of VAL78HA:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS77	0.00	1.00
VAL78	0.80	1.00
PHE79	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K77HA	1.00
V78HG11	1.00
V78HG21	1.00
V78H	1.00
V78HB	1.00
V78HA	1.00
F79H	1.00
F79HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS77	HA	1.00	0.136	0.00	0.00
VAL78	HA	1.00	0.001	1.00	2.12
VAL78	HB	1.00	0.003	1.00	0.21
VAL78	HG11	1.00	0.000	1.00	0.70
VAL78	HG21	1.00	0.619	0.00	0.00
VAL78	H	1.00	0.006	1.00	-251004.00
PHE79	HA	1.00	0.014	1.00	0.12
PHE79	H	1.00	0.004	1.00	-1444837.00

3.78.7 Detailed Probabilities of VAL78HB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL78	1.00	1.00
PHE79	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V78HA	1.00
V78HG11	1.00
V78HG21	1.00
V78H	1.00
V78HB	1.00
F79H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL78	HA	1.00	0.000	1.00	0.28
VAL78	HB	1.00	0.005	1.00	3.52
VAL78	HG11	1.00	0.002	1.00	1.60
VAL78	HG21	1.00	0.003	1.00	1.54
VAL78	H	1.00	0.010	1.00	-670087.00
PHE79	H	1.00	0.009	1.00	-177253.00

3.78.8 Detailed Probabilities of VAL78HG11:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL78	0.80	1.00
PHE79	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V78HA	1.00
V78HG12	1.00
V78HG21	1.00
V78H	1.00
V78HB	1.00
F79H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL78	HA	1.00	0.006	1.00	0.54
VAL78	HB	1.00	0.001	1.00	1.07
VAL78	HG11	1.00	0.119	0.00	0.00
VAL78	HG21	1.00	0.005	1.00	2.76
VAL78	H	1.00	0.000	1.00	-354862.00
PHE79	H	0.98	0.001	1.00	-714021.00
PHE79	HA	0.60	0.021	1.00	0.21

3.78.9 Detailed Probabilities of VAL78HG21:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL78	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V78HA	1.00
V78HG11	1.00
V78HG22	1.00
V78H	1.00
V78HB	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL78	HA	1.00	0.003	1.00	0.55
VAL78	HB	1.00	0.003	1.00	1.14
VAL78	HG11	1.00	0.009	1.00	4.37
VAL78	HG21	1.00	0.005	1.00	46.27
VAL78	H	1.00	0.002	1.00	-648934.00

3.78.10 Detailed Probabilities of VAL78H:

Overall probability: 0.671

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS77	0.63	1.00
VAL78	0.80	1.00
PHE79	0.52	1.00

Expected NOESY Contacts

Proton	Expected probability
K77HG2	0.98
K77HG3	0.96
K77HA	1.00
K77HB3	1.00
K77HB2	1.00
K77H	1.00
V78HA	1.00
V78HG11	1.00
V78HG21	1.00
V78HB	1.00
V78H	1.00
F79H	1.00
F79HA	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS77	HA	1.00	0.006	1.00	1.39
LYS77	HB2	1.00	0.467	0.00	0.00
LYS77	HB3	1.00	0.467	0.00	0.00
LYS77	HG2	0.98	0.228	0.02	0.00
LYS77	HG3	0.96	0.004	1.00	0.16
LYS77	H	1.00	0.005	1.00	-100425.00
LYS77	HD2	0.56	0.005	1.00	0.37
LYS77	HD3	0.58	0.005	1.00	0.37
VAL78	HA	1.00	0.009	1.00	0.16
VAL78	HB	1.00	0.005	1.00	0.54
VAL78	HG11	1.00	0.546	0.00	0.00
VAL78	HG21	1.00	0.004	1.00	0.71
VAL78	H	1.00	0.004	1.00	-4592120.00
PHE79	HA	0.96	0.148	0.04	0.00
PHE79	H	1.00	0.005	1.00	-76142.00

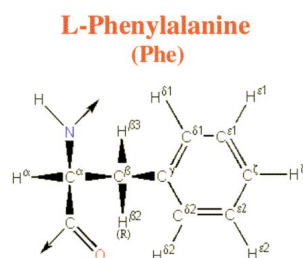
3.79 PHE(79)

Figure 78: 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	173.357	175.508	2.010	0.000	0.000
CA 3.79.1	55.953	58.245	3.808	0.822	1.000
CB 3.79.2	40.184	40.078	3.616	1.000	1.000
CD 3.79.3	131.806	131.234	9.579	1.000	1.000
CE1 3.79.4	130.139	130.599	3.219	1.000	1.000
CE2 3.79.5	130.226	130.633	2.839	1.000	1.000
CZ 3.79.6	128.170	129.042	3.448	0.750	1.000
N 3.79.7	126.174	120.315	4.931	1.000	1.000
HA 3.79.8	4.567	4.625	1.237	0.909	1.000
HB2 3.79.9	1.042	2.980	0.399	1.000	1.000
HB3 3.79.10	2.075	2.916	0.434	1.000	1.000
HD 3.79.11	6.720	7.037	0.347	0.875	1.000
HE1 3.79.12	7.097	7.046	0.417	1.000	1.000
HE2 3.79.13	7.097	7.043	0.400	1.000	1.000
HZ 3.79.14	6.990	6.984	1.598	1.000	1.000
H 3.79.15	8.374	8.375	0.710	0.700	1.000

3.79.1 Detailed Probabilities of PHE79CA:

Overall probability: 0.822

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL78	0.68	1.00
PHE79	0.83	1.00
LEU80	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V78HA	1.00
V78H	0.96
F79HB2	1.00
F79HB3	1.00
F79HD1	1.00
F79H	1.00
F79HA	1.00
L80HA	1.00
L80H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL78	HA	1.00	0.014	1.00	0.12
VAL78	H	0.96	0.148	0.04	0.00
VAL78	HG11	0.61	0.021	1.00	0.21
PHE79	HA	1.00	0.016	1.00	90.61
PHE79	HB2	1.00	0.006	1.00	0.36
PHE79	HB3	1.00	0.018	1.00	0.98
PHE79	HD1	1.00	0.022	1.00	0.06
PHE79	H	1.00	0.043	0.00	0.00
PHE79	HE1	0.74	0.004	1.00	0.18
LEU80	HA	1.00	0.004	1.00	0.08
LEU80	H	1.00	0.002	1.00	0.95

3.79.2 Detailed Probabilities of PHE79CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE79	1.00	1.00
LEU80	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F79HA	1.00
F79HB3	1.00
F79HD1	1.00
F79HE2	1.00
F79H	1.00
F79HB2	1.00
L80H	1.00

NOESY contacts detailed probability

3.79 PHE(79)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE79	HA	1.00	0.001	1.00	0.16
PHE79	HB2	1.00	0.012	1.00	0.57
PHE79	HB3	1.00	0.000	1.00	0.53
PHE79	HD1	1.00	0.001	1.00	0.25
PHE79	HE2	1.00	0.028	1.00	0.07
PHE79	H	1.00	0.004	1.00	0.12
PHE79	HE1	0.90	0.028	1.00	0.07
LEU80	H	1.00	0.007	1.00	0.08

3.79.3 Detailed Probabilities of PHE79CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE79	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F79HA	1.00
F79HB2	1.00
F79HB3	1.00
F79HD2	1.00
F79HE1	1.00
F79HE2	1.00
F79HZ	1.00
F79H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE79	HA	1.00	0.004	1.00	0.55
PHE79	HB2	1.00	0.023	1.00	1.17
PHE79	HB3	1.00	0.010	1.00	1.13
PHE79	HD1	1.00	0.003	1.00	13.56
PHE79	HE1	1.00	0.006	1.00	3.01
PHE79	HE2	1.00	0.006	1.00	3.01
PHE79	HZ	1.00	0.009	1.00	0.48
PHE79	H	0.99	0.004	1.00	0.56

3.79.4 Detailed Probabilities of PHE79CE1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE79	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F79HD1	1.00
F79HE2	1.00
F79HZ	1.00
F79HE1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE79	HD1	1.00	0.004	1.00	2.44
PHE79	HE1	1.00	0.009	1.00	15.02
PHE79	HE2	1.00	0.009	1.00	15.02
PHE79	HZ	1.00	0.026	1.00	2.55
PHE79	HB3	0.89	0.013	1.00	0.25

3.79.5 Detailed Probabilities of PHE79CE2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE79	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F79HB2	1.00
F79HB3	1.00
F79HD1	1.00
F79HE1	1.00
F79HZ	1.00
F79HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE79	HB2	1.00	0.030	1.00	0.00
PHE79	HB3	1.00	0.013	1.00	0.25
PHE79	HD1	1.00	0.004	1.00	2.44
PHE79	HE1	1.00	0.009	1.00	15.02
PHE79	HE2	1.00	0.009	1.00	15.02
PHE79	HZ	1.00	0.026	1.00	2.55

3.79.6 Detailed Probabilities of PHE79CZ:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE79	0.75	1.00

Expected NOESY Contacts

Proton	Expected probability
F79HD1	1.00
F79HE1	1.00
F79HE2	1.00
F79HZ	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE79	HD1	1.00	0.278	0.00	0.00
PHE79	HE1	1.00	0.000	1.00	2.04
PHE79	HE2	1.00	0.000	1.00	2.04
PHE79	HZ	1.00	0.008	1.00	6.79

3.79.7 Detailed Probabilities of PHE79N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL78	1.00	1.00
PHE79	1.00	1.00
LEU80	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V78H	1.00
V78HG13	0.98
V78HB	1.00
V78HA	1.00
F79HA	1.00
F79HB2	1.00
F79HB3	1.00
F79HD1	1.00
F79H	1.00
L80H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL78	HA	1.00	0.004	1.00	-1444837.00
VAL78	HB	1.00	0.009	1.00	-177253.00
VAL78	HG11	0.98	0.001	1.00	-714021.00
VAL78	H	1.00	0.005	1.00	-76142.00
VAL78	HG21	0.95	0.004	1.00	-498022.00
PHE79	HA	1.00	0.004	1.00	-275808.00
PHE79	HB2	1.00	0.012	1.00	-198086.00
PHE79	HB3	1.00	0.002	1.00	-291537.00
PHE79	HD1	1.00	0.003	1.00	-341985.00
PHE79	H	1.00	0.002	1.00	-3717956.00
LEU80	H	1.00	0.001	1.00	-131885.00

3.79.8 Detailed Probabilities of PHE79HA:

Overall probability: 0.909

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL78	1.00	1.00
PHE79	1.00	1.00
LEU80	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
V78HA	1.00
V78H	0.96
F79HB2	1.00
F79HB3	1.00
F79HD1	1.00
F79H	1.00
F79HA	1.00
L80HA	1.00
L80H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL78	HA	1.00	0.018	1.00	0.06
VAL78	H	0.96	0.019	1.00	-1716215.00
VAL78	HB	0.85	0.015	1.00	0.17
VAL78	HG11	0.61	0.009	1.00	0.22
PHE79	HA	1.00	0.016	1.00	90.61
PHE79	HB2	1.00	0.001	1.00	0.16
PHE79	HB3	1.00	0.001	1.00	0.17
PHE79	HD1	1.00	0.004	1.00	0.55
PHE79	H	1.00	0.004	1.00	-275808.00
LEU80	HA	1.00	0.627	0.00	0.00
LEU80	H	1.00	0.000	1.00	-931742.00

3.79.9 Detailed Probabilities of PHE79HB2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE79	1.00	1.00
LEU80	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F79HA	1.00
F79HB3	1.00
F79HD1	1.00
F79HE2	1.00
F79H	1.00
F79HB2	1.00
L80H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE79	HA	1.00	0.006	1.00	0.36
PHE79	HB2	1.00	0.012	1.00	0.57
PHE79	HB3	1.00	0.010	1.00	0.59
PHE79	HD1	1.00	0.023	1.00	1.17
PHE79	HE2	1.00	0.030	1.00	0.00
PHE79	H	1.00	0.012	1.00	-198086.00
LEU80	H	1.00	0.016	1.00	-112842.00

3.79.10 Detailed Probabilities of PHE79HB3:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE79	1.00	1.00
LEU80	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F79HA	1.00
F79HB2	1.00
F79HD1	1.00
F79HE2	1.00
F79H	1.00
F79HB3	1.00
L80H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE79	HA	1.00	0.018	1.00	0.98
PHE79	HB2	1.00	0.000	1.00	0.53
PHE79	HB3	1.00	0.001	1.00	0.62
PHE79	HD1	1.00	0.010	1.00	1.13
PHE79	HE2	1.00	0.013	1.00	0.25
PHE79	H	1.00	0.002	1.00	-291537.00
PHE79	HE1	0.89	0.013	1.00	0.25
LEU80	H	1.00	0.001	1.00	-221876.00

3.79.11 Detailed Probabilities of PHE79HD1:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE79	0.88	1.00

Expected NOESY Contacts

Proton	Expected probability
F79HA	1.00
F79HB2	1.00
F79HB3	1.00
F79HD2	1.00
F79HE1	1.00
F79HE2	1.00
F79HZ	1.00
F79H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE79	HA	1.00	0.022	1.00	0.06
PHE79	HB2	1.00	0.001	1.00	0.25
PHE79	HB3	1.00	0.001	1.00	0.30
PHE79	HD1	1.00	0.003	1.00	13.56
PHE79	HE1	1.00	0.004	1.00	2.44
PHE79	HE2	1.00	0.004	1.00	2.44
PHE79	HZ	1.00	0.278	0.00	0.00
PHE79	H	0.99	0.003	1.00	-341985.00

3.79.12 Detailed Probabilities of PHE79HE1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE79	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F79HD1	1.00
F79HE2	1.00
F79HZ	1.00
F79HE1	1.00

NOESY contacts detailed probability

3.79 PHE(79)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE79	HD1	1.00	0.006	1.00	3.01
PHE79	HE1	1.00	0.009	1.00	15.02
PHE79	HE2	1.00	0.009	1.00	15.02
PHE79	HZ	1.00	0.000	1.00	2.04
PHE79	HA	0.74	0.004	1.00	0.18
PHE79	HB2	0.90	0.028	1.00	0.07
PHE79	HB3	0.89	0.014	1.00	0.07

3.79.13 Detailed Probabilities of PHE79HE2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE79	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F79HB2	1.00
F79HB3	1.00
F79HD1	1.00
F79HE1	1.00
F79HZ	1.00
F79HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE79	HB2	1.00	0.028	1.00	0.07
PHE79	HB3	1.00	0.014	1.00	0.07
PHE79	HD1	1.00	0.006	1.00	3.01
PHE79	HE1	1.00	0.009	1.00	15.02
PHE79	HE2	1.00	0.009	1.00	15.02
PHE79	HZ	1.00	0.000	1.00	2.04

3.79.14 Detailed Probabilities of PHE79HZ:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE79	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F79HD1	1.00
F79HE1	1.00
F79HE2	1.00
F79HZ	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE79	HD1	1.00	0.009	1.00	0.48
PHE79	HE1	1.00	0.026	1.00	2.55
PHE79	HE2	1.00	0.026	1.00	2.55
PHE79	HZ	1.00	0.008	1.00	6.79

3.79.15 Detailed Probabilities of PHE79H:

Overall probability: 0.700

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL78	0.75	1.00
PHE79	0.80	1.00
LEU80	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V78H	1.00
V78HG13	0.98
V78HB	1.00
V78HA	1.00
F79HA	1.00
F79HB2	1.00
F79HB3	1.00
F79HD1	1.00
F79H	1.00
L80H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL78	HA	1.00	0.005	1.00	1.16
VAL78	HB	1.00	0.006	1.00	0.10
VAL78	HG11	0.98	0.002	1.00	0.63
VAL78	H	1.00	0.051	0.00	0.00
PHE79	HA	1.00	0.043	0.00	0.00
PHE79	HB2	1.00	0.004	1.00	0.12
PHE79	HB3	1.00	0.007	1.00	0.16
PHE79	HD1	1.00	0.004	1.00	0.56
PHE79	H	1.00	0.002	1.00	-3717956.00
LEU80	H	1.00	0.230	0.00	0.00

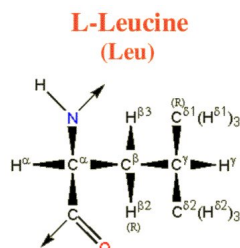
3.80 LEU(80)

Figure 79: Image from the BMRB

Residue probability: 0.789

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	173.503	177.056	1.929	0.000	0.000
CA 3.80.1	53.998	55.735	3.802	0.700	1.000
CB 3.80.2	45.667	42.389	3.750	0.850	1.000
CG 3.80.3	28.308	26.892	3.086	0.375	1.000
CD1 3.80.4	25.505	24.837	3.657	0.714	1.000
CD2 3.80.5	27.658	24.201	3.117	1.000	1.000
N 3.80.6	123.959	121.785	4.943	0.862	1.000
HA 3.80.7	5.546	4.315	0.840	1.000	1.000
HB2 3.80.8	1.753	1.601	0.373	0.556	1.000
HB3 3.80.9	1.288	1.508	0.398	0.625	1.000
HG 3.80.10	1.441	1.510	0.340	1.000	1.000
HD1 3.80.11	0.775	0.739	0.294	0.857	1.000
HD2 3.80.12	0.776	0.727	0.421	0.857	1.000
H 3.80.13	8.601	8.237	0.647	0.857	1.000

3.80.1 Detailed Probabilities of LEU80CA:

Overall probability: 0.700

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE79	0.00	1.00
LEU80	0.71	1.00
LEU81	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F79HA	1.00
L80HB2	1.00
L80HB3	1.00
L80HG	1.00
L80HD11	0.99
L80HD21	0.99
L80H	1.00
L80HA	1.00
L81H	1.00
L81HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE79	HA	1.00	0.627	0.00	0.00
LEU80	HA	1.00	0.020	1.00	3.39
LEU80	HB2	1.00	0.177	0.00	0.00
LEU80	HB3	1.00	0.004	1.00	0.32
LEU80	HG	1.00	0.026	1.00	0.52
LEU80	HD11	0.99	0.001	1.00	0.98
LEU80	HD21	0.99	0.000	1.00	0.98
LEU80	H	1.00	0.465	0.00	0.00
LEU81	HA	1.00	0.012	1.00	0.13
LEU81	H	1.00	0.003	1.00	1.18

3.80.2 Detailed Probabilities of LEU80CB:

Overall probability: 0.850

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU80	1.00	1.00
LEU81	0.32	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
L81H	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	0.002	1.00	0.26
LEU80	HB2	1.00	0.010	1.00	2.14
LEU80	HB3	1.00	0.024	1.00	1.49
LEU80	HG	1.00	0.003	1.00	0.62
LEU80	HD11	1.00	0.004	1.00	1.17
LEU80	HD21	1.00	0.003	1.00	1.17
LEU80	H	1.00	0.003	1.00	0.37
LEU81	H	1.00	0.048	0.00	0.00
LEU81	HA	0.65	0.034	0.65	0.00

3.80.3 Detailed Probabilities of LEU80CG:

Overall probability: 0.375

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU80	0.29	1.00
LEU81	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
L81H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU80	HA	1.00	0.001	1.00	0.12
LEU80	HB2	1.00	0.061	0.00	0.00
LEU80	HB3	1.00	0.171	0.00	0.00
LEU80	HG	1.00	0.018	1.00	12.32
LEU80	HD11	1.00	0.055	0.00	0.00
LEU80	HD21	1.00	0.056	0.00	0.00
LEU80	H	1.00	0.055	0.00	0.00
LEU81	H	0.98	0.019	1.00	0.21

3.80.4 Detailed Probabilities of LEU80CD1:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU80	0.71	1.00

Expected NOESY Contacts

Proton	Expected probability
L80HA	0.99
L80HB2	1.00
L80HB3	1.00
L80HG	1.00
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	0.005	1.00	0.66
LEU80	HB2	1.00	0.135	0.00	0.00
LEU80	HB3	1.00	0.083	0.00	0.00
LEU80	HG	1.00	0.013	1.00	3.62
LEU80	HD11	1.00	0.022	1.00	119.01
LEU80	HD21	1.00	0.023	1.00	119.01
LEU80	H	0.86	0.028	1.00	0.27

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	0.004	1.00	0.13
LEU80	HB2	1.00	0.008	1.00	0.71
LEU80	HB3	1.00	0.014	1.00	0.56
LEU80	HG	1.00	0.009	1.00	1.07
LEU80	HD11	1.00	0.005	1.00	32.30
LEU80	HD21	1.00	0.004	1.00	32.30
LEU80	H	0.85	0.001	1.00	0.08

3.80.6 Detailed Probabilities of LEU80N:

Overall probability: 0.862

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE79	0.80	1.00
LEU80	1.00	1.00
LEU81	0.64	1.00

Expected NOESY Contacts

Proton	Expected probability
F79HB2	1.00
F79H	1.00
F79HB3	1.00
F79HA	1.00
L80HA	1.00
L80HB2	1.00
L80HB3	1.00
L80HG	1.00
L80H	1.00
L81H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE79	HA	1.00	0.000	1.00	-931742.00
PHE79	HB2	1.00	0.016	1.00	-112842.00
PHE79	HB3	1.00	0.001	1.00	-221876.00
PHE79	H	1.00	0.230	0.00	0.00
PHE79	HD1	0.77	0.004	1.00	-72935.00
LEU80	HA	1.00	0.000	1.00	-211200.00
LEU80	HB2	1.00	0.003	1.00	-476455.00
LEU80	HB3	1.00	0.000	1.00	-349050.00
LEU80	HG	1.00	0.020	1.00	-273862.00
LEU80	H	1.00	0.003	1.00	-3584513.00
LEU80	HD11	0.88	0.003	1.00	-326912.00
LEU80	HD21	0.87	0.002	1.00	-326912.00
LEU81	H	1.00	0.459	0.00	0.00
LEU81	HA	0.93	0.032	0.93	0.00
LEU81	HB2	0.64	0.013	1.00	-198518.00

3.80.7 Detailed Probabilities of LEU80HA:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE79	1.00	1.00
LEU80	1.00	1.00
LEU81	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F79HA	1.00
L80HB2	1.00
L80HB3	1.00
L80HG	1.00
L80HD11	0.99
L80HD21	0.99
L80H	1.00
L80HA	1.00
L81H	1.00
L81HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE79	HA	1.00	0.004	1.00	0.08
LEU80	HA	1.00	0.020	1.00	3.39
LEU80	HB2	1.00	0.002	1.00	0.26
LEU80	HB3	1.00	0.005	1.00	0.28
LEU80	HG	1.00	0.001	1.00	0.12
LEU80	HD11	0.99	0.005	1.00	0.66
LEU80	HD21	0.99	0.004	1.00	0.13
LEU80	H	1.00	0.000	1.00	-211200.00
LEU81	HA	1.00	0.015	1.00	0.14
LEU81	H	1.00	0.003	1.00	-1579949.00

3.80.8 Detailed Probabilities of LEU80HB2:

Overall probability: 0.556

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU80	0.43	1.00
LEU81	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
L81H	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	0.177	0.00	0.00
LEU80	HB2	1.00	0.010	1.00	2.14
LEU80	HB3	1.00	0.309	0.00	0.00
LEU80	HG	1.00	0.061	0.00	0.00
LEU80	HD11	1.00	0.135	0.00	0.00
LEU80	HD21	1.00	0.008	1.00	0.71
LEU80	H	1.00	0.003	1.00	-476455.00
LEU81	H	1.00	0.006	1.00	-200418.00
LEU81	HA	0.65	0.003	1.00	0.14

3.80.9 Detailed Probabilities of LEU80HB3:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU80	0.71	1.00
LEU81	0.00	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
L81H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU80	HA	1.00	0.004	1.00	0.32
LEU80	HB2	1.00	0.024	1.00	1.49
LEU80	HB3	1.00	0.002	1.00	1.66
LEU80	HG	1.00	0.171	0.00	0.00
LEU80	HD11	1.00	0.083	0.00	0.00
LEU80	HD21	1.00	0.014	1.00	0.56
LEU80	H	1.00	0.000	1.00	-349050.00
LEU81	H	1.00	0.058	0.00	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
LEU81	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
L81H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU80	HA	1.00	0.026	1.00	0.52
LEU80	HB2	1.00	0.003	1.00	0.62
LEU80	HB3	1.00	0.003	1.00	0.57
LEU80	HG	1.00	0.018	1.00	12.32
LEU80	HD11	1.00	0.013	1.00	3.62
LEU80	HD21	1.00	0.009	1.00	1.07
LEU80	H	1.00	0.020	1.00	-273862.00
LEU81	H	0.98	0.022	1.00	-352536.00

3.80.11 Detailed Probabilities of LEU80HD11:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU80	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
L80HA	0.99
L80HB2	1.00
L80HB3	1.00
L80HG	1.00
L80HD12	1.00
L80HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU80	HA	0.99	0.001	1.00	0.98
LEU80	HB2	1.00	0.004	1.00	1.17
LEU80	HB3	1.00	0.003	1.00	1.07
LEU80	HG	1.00	0.055	0.00	0.00
LEU80	HD11	1.00	0.022	1.00	119.01
LEU80	HD21	1.00	0.005	1.00	32.30
LEU80	H	0.86	0.003	1.00	-326912.00

3.80.12 Detailed Probabilities of LEU80HD21:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU80	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
L80HA	0.99
L80HB2	1.00
L80HB3	1.00
L80HG	1.00
L80HD11	1.00
L80HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU80	HA	0.99	0.000	1.00	0.98
LEU80	HB2	1.00	0.003	1.00	1.17
LEU80	HB3	1.00	0.002	1.00	1.07
LEU80	HG	1.00	0.056	0.00	0.00
LEU80	HD11	1.00	0.023	1.00	119.01
LEU80	HD21	1.00	0.004	1.00	32.30
LEU80	H	0.85	0.002	1.00	-326912.00

3.80.13 Detailed Probabilities of LEU80H:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE79	1.00	1.00
LEU80	0.71	1.00
LEU81	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F79HB2	1.00
F79H	1.00
F79HB3	1.00
F79HA	1.00
L80HA	1.00
L80HB2	1.00
L80HB3	1.00
L80HG	1.00
L80H	1.00
L81H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE79	HA	1.00	0.002	1.00	0.95
PHE79	HB2	1.00	0.007	1.00	0.08
PHE79	HB3	1.00	0.003	1.00	0.07
PHE79	H	1.00	0.001	1.00	-131885.00
PHE79	HD1	0.77	0.015	1.00	0.17
LEU80	HA	1.00	0.465	0.00	0.00
LEU80	HB2	1.00	0.003	1.00	0.37
LEU80	HB3	1.00	0.003	1.00	0.31
LEU80	HG	1.00	0.055	0.00	0.00
LEU80	H	1.00	0.003	1.00	-3584513.00
LEU80	HD11	0.88	0.028	1.00	0.27
LEU80	HD21	0.87	0.001	1.00	0.08
LEU81	H	1.00	0.022	1.00	-219742.00
LEU81	HB2	0.64	0.020	1.00	0.07

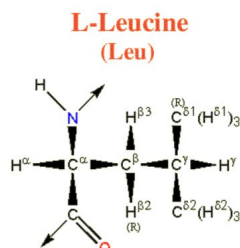


Figure 80: Image from the BMRB

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	173.649	177.056	1.929	0.000	0.000
CA 3.81.1	53.064	55.735	3.802	1.000	1.000
CB 3.81.2	45.777	42.389	3.750	0.800	1.000
CG 3.81.3	27.360	26.892	3.086	0.875	1.000
CD1 3.81.4	24.934	24.837	3.657	0.833	1.000
CD2 3.81.5	25.856	24.201	3.117	0.429	1.000
N 3.81.6	126.694	121.785	4.943	0.929	1.000
HA 3.81.7	5.269	4.315	0.840	0.900	1.000
HB2 3.81.8	1.919	1.601	0.373	0.875	1.000
HB3 3.81.9	1.356	1.508	0.398	0.875	1.000
HG 3.81.10	1.346	1.510	0.340	0.875	1.000
HD1 3.81.11	0.789	0.739	0.294	0.571	1.000
HD2 3.81.12	0.706	0.727	0.421	0.400	1.000
H 3.81.13	9.063	8.237	0.647	0.643	1.000

3.81.1 Detailed Probabilities of LEU81CA:

Overall probability: 1.000
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU80	1.00	1.00
LEU81	1.00	1.00
LEU82	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L80HA	1.00
L81HB2	1.00
L81HB3	1.00
L81HG	1.00
L81HD11	0.99
L81HD21	0.99
L81H	1.00
L81HA	1.00
L82H	1.00
L82HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU80	HA	1.00	0.015	1.00	0.14
LEU80	HB2	0.65	0.003	1.00	0.14
LEU81	HA	1.00	0.002	1.00	2.06
LEU81	HB2	1.00	0.006	1.00	0.21
LEU81	HB3	1.00	0.005	1.00	0.48
LEU81	HG	1.00	0.005	1.00	0.48
LEU81	HD11	0.99	0.010	1.00	0.47
LEU81	HD21	0.99	0.007	1.00	0.22
LEU81	H	1.00	0.001	1.00	0.16
LEU82	HA	1.00	0.000	1.00	0.11
LEU82	H	1.00	0.005	1.00	0.88

3.81.2 Detailed Probabilities of LEU81CB:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU81	0.77	1.00
LEU82	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L81HA	1.00
L81HB3	1.00
L81HG	1.00
L81HD11	1.00
L81HD21	1.00
L81H	1.00
L81HB2	1.00
L82H	1.00

NOESY contacts detailed probability

3.81 LEU(81)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU81	HA	1.00	0.002	1.00	0.20
LEU81	HB2	1.00	0.006	1.00	0.94
LEU81	HB3	1.00	0.004	1.00	1.42
LEU81	HG	1.00	0.006	1.00	1.42
LEU81	HD11	1.00	0.047	0.00	0.00
LEU81	HD21	1.00	0.036	0.40	0.00
LEU81	H	1.00	0.006	1.00	0.23
LEU82	H	1.00	0.009	1.00	0.06

3.81.3 Detailed Probabilities of LEU81CG:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU81	0.86	1.00
LEU82	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L81HA	1.00
L81HB2	1.00
L81HB3	1.00
L81HD11	1.00
L81HD21	1.00
L81H	1.00
L81HG	1.00
L82H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU81	HA	1.00	0.001	1.00	0.33
LEU81	HB2	1.00	0.005	1.00	0.75
LEU81	HB3	1.00	0.004	1.00	6.05
LEU81	HG	1.00	0.006	1.00	6.05
LEU81	HD11	1.00	0.021	1.00	1.84
LEU81	HD21	1.00	0.062	0.00	0.00
LEU81	H	1.00	0.011	1.00	0.15
LEU82	H	0.98	0.006	1.00	0.18

3.81.4 Detailed Probabilities of LEU81CD1:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU81	0.83	1.00

Expected NOESY Contacts

Proton	Expected probability
L81HA	0.99
L81HB2	1.00
L81HB3	1.00
L81HG	1.00
L81HD12	1.00
L81HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU81	HA	0.99	0.000	1.00	1.30
LEU81	HB2	1.00	0.025	1.00	1.84
LEU81	HB3	1.00	0.015	1.00	3.41
LEU81	HG	1.00	0.025	1.00	3.41
LEU81	HD11	1.00	0.005	1.00	196.23
LEU81	HD21	1.00	0.425	0.00	0.00

3.81.5 Detailed Probabilities of LEU81CD2:

Overall probability: 0.429

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU81	0.43	1.00

Expected NOESY Contacts

Proton	Expected probability
L81HA	0.99
L81HB2	1.00
L81HB3	1.00
L81HG	1.00
L81HD11	1.00
L81HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU81	HA	0.99	0.030	1.00	0.00
LEU81	HB2	1.00	0.040	0.00	0.00
LEU81	HB3	1.00	0.087	0.00	0.00
LEU81	HG	1.00	0.097	0.00	0.00
LEU81	HD11	1.00	0.057	0.00	0.00
LEU81	HD21	1.00	0.021	1.00	164.25
LEU81	H	0.85	0.024	1.00	0.29

3.81.6 Detailed Probabilities of LEU81N:

Overall probability: 0.929

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU80	0.86	1.00
LEU81	1.00	1.00
LEU82	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L80HB3	1.00
L80HB2	1.00
L80HA	1.00
L80H	1.00
L80HG	0.98
L81HA	1.00
L81HB2	1.00
L81HB3	1.00
L81HG	1.00
L81H	1.00
L82H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU80	HA	1.00	0.003	1.00	-1579949.00
LEU80	HB2	1.00	0.006	1.00	-200418.00
LEU80	HB3	1.00	0.058	0.00	0.00
LEU80	HG	0.98	0.022	1.00	-352536.00
LEU80	H	1.00	0.022	1.00	-219742.00
LEU80	HD11	0.53	0.004	1.00	-1191278.00
LEU80	HD21	0.58	0.005	1.00	-1191278.00
LEU81	HA	1.00	0.006	1.00	-310552.00
LEU81	HB2	1.00	0.004	1.00	-455169.00
LEU81	HB3	1.00	0.010	1.00	-491205.00
LEU81	HG	1.00	0.000	1.00	-491205.00
LEU81	H	1.00	0.004	1.00	-4053824.00
LEU81	HD11	0.88	0.018	1.00	-1191278.00
LEU82	H	1.00	0.013	1.00	-118622.00

3.81.7 Detailed Probabilities of LEU81HA:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU80	1.00	1.00
LEU81	1.00	1.00
LEU82	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
L80HA	1.00
L81HB2	1.00
L81HB3	1.00
L81HG	1.00
L81HD11	0.99
L81HD21	0.99
L81H	1.00
L81HA	1.00
L82H	1.00
L82HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU80	HA	1.00	0.012	1.00	0.13
LEU81	HA	1.00	0.002	1.00	2.06
LEU81	HB2	1.00	0.002	1.00	0.20
LEU81	HB3	1.00	0.002	1.00	0.31
LEU81	HG	1.00	0.001	1.00	0.33
LEU81	HD11	0.99	0.000	1.00	1.30
LEU81	HD21	0.99	0.030	1.00	0.00
LEU81	H	1.00	0.006	1.00	-310552.00
LEU82	HA	1.00	0.048	0.00	0.00
LEU82	H	1.00	0.001	1.00	-1621019.00

3.81.8 Detailed Probabilities of LEU81HB2:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU81	0.86	1.00
LEU82	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L81HA	1.00
L81HB3	1.00
L81HG	1.00
L81HD11	1.00
L81HD21	1.00
L81H	1.00
L81HB2	1.00
L82H	1.00

NOESY contacts detailed probability

3.81 LEU(81)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU81	HA	1.00	0.006	1.00	0.21
LEU81	HB2	1.00	0.006	1.00	0.94
LEU81	HB3	1.00	0.005	1.00	0.94
LEU81	HG	1.00	0.005	1.00	0.75
LEU81	HD11	1.00	0.025	1.00	1.84
LEU81	HD21	1.00	0.040	0.00	0.00
LEU81	H	1.00	0.004	1.00	-455169.00
LEU82	H	1.00	0.004	1.00	-134613.00

3.81.9 Detailed Probabilities of LEU81HB3:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU81	0.86	1.00
LEU82	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L81HA	1.00
L81HB2	1.00
L81HG	1.00
L81HD11	1.00
L81HD21	1.00
L81H	1.00
L81HB3	1.00
L82H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU81	HA	1.00	0.005	1.00	0.48
LEU81	HB2	1.00	0.004	1.00	1.42
LEU81	HB3	1.00	0.029	1.00	1.91
LEU81	HG	1.00	0.004	1.00	6.05
LEU81	HD11	1.00	0.015	1.00	3.41
LEU81	HD21	1.00	0.087	0.00	0.00
LEU81	H	1.00	0.010	1.00	-491205.00
LEU82	H	1.00	0.005	1.00	-399450.00

3.81.10 Detailed Probabilities of LEU81HG:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU81	0.86	1.00
LEU82	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L81HA	1.00
L81HB2	1.00
L81HB3	1.00
L81HD11	1.00
L81HD21	1.00
L81H	1.00
L81HG	1.00
L82H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU81	HA	1.00	0.005	1.00	0.48
LEU81	HB2	1.00	0.006	1.00	1.42
LEU81	HB3	1.00	0.019	1.00	1.91
LEU81	HG	1.00	0.006	1.00	6.05
LEU81	HD11	1.00	0.025	1.00	3.41
LEU81	HD21	1.00	0.097	0.00	0.00
LEU81	H	1.00	0.000	1.00	-491205.00
LEU82	H	0.98	0.005	1.00	-399450.00

3.81.11 Detailed Probabilities of LEU81HD11:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU81	0.57	1.00

Expected NOESY Contacts

Proton	Expected probability
L81HA	0.99
L81HB2	1.00
L81HB3	1.00
L81HG	1.00
L81HD12	1.00
L81HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU81	HA	0.99	0.010	1.00	0.47
LEU81	HB2	1.00	0.047	0.00	0.00
LEU81	HB3	1.00	0.538	0.00	0.00
LEU81	HG	1.00	0.021	1.00	1.84
LEU81	HD11	1.00	0.005	1.00	196.23
LEU81	HD21	1.00	0.057	0.00	0.00
LEU81	H	0.86	0.018	1.00	-1191278.00

3.81.12 Detailed Probabilities of LEU81HD21:

Overall probability: 0.400

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU81	0.40	1.00

Expected NOESY Contacts

Proton	Expected probability
L81HA	0.99
L81HB2	1.00
L81HB3	1.00
L81HG	1.00
L81HD11	1.00
L81HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU81	HA	0.99	0.007	1.00	0.22
LEU81	HB2	1.00	0.036	0.40	0.00
LEU81	HB3	1.00	0.621	0.00	0.00
LEU81	HG	1.00	0.062	0.00	0.00
LEU81	HD11	1.00	0.425	0.00	0.00
LEU81	HD21	1.00	0.021	1.00	164.25

3.81.13 Detailed Probabilities of LEU81H:

Overall probability: 0.643

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU80	0.57	1.00
LEU81	0.83	1.00
LEU82	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L80HB3	1.00
L80HB2	1.00
L80HA	1.00
L80H	1.00
L80HG	0.98
L81HA	1.00
L81HB2	1.00
L81HB3	1.00
L81HG	1.00
L81H	1.00
L82H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU80	HA	1.00	0.003	1.00	1.18
LEU80	HB2	1.00	0.048	0.00	0.00
LEU80	HB3	1.00	0.182	0.00	0.00
LEU80	HG	0.98	0.019	1.00	0.21
LEU80	H	1.00	0.459	0.00	0.00
LEU80	HD11	0.53	0.007	1.00	0.55
LEU80	HD21	0.58	0.014	1.00	0.06
LEU81	HA	1.00	0.001	1.00	0.16
LEU81	HB2	1.00	0.006	1.00	0.23
LEU81	HB3	1.00	0.043	0.00	0.00
LEU81	HG	1.00	0.011	1.00	0.15
LEU81	H	1.00	0.004	1.00	-4053824.00
LEU81	HD21	0.87	0.024	1.00	0.29
LEU82	H	1.00	0.087	0.00	0.00

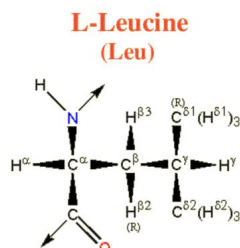
3.82 LEU(82)

Figure 81: Image from the BMRB

Residue probability: 0.616

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.479	177.056	1.929	0.000	0.000
CA 3.82.1	53.135	55.735	3.802	0.360	1.000
CB 3.82.2	44.222	42.389	3.750	0.838	1.000
CG 3.82.3	26.760	26.892	3.086	0.777	1.000
CD1 3.82.4	26.011	24.837	3.657	0.001	1.000
CD2 3.82.5	23.860	24.201	3.117	0.500	1.000
N 3.82.6	124.888	121.785	4.943	0.929	1.000
HA 3.82.7	4.911	4.315	0.840	0.701	1.000
HB2 3.82.8	1.621	1.601	0.373	0.500	1.000
HB3 3.82.9	1.736	1.508	0.398	0.750	1.000
HG 3.82.10	1.598	1.510	0.340	0.400	1.000
HD1 3.82.11	0.778	0.739	0.294	0.657	1.000
HD2 3.82.12	0.825	0.727	0.421	0.667	1.000
H 3.82.13	8.864	8.237	0.647	0.923	1.000

3.82.1 Detailed Probabilities of LEU82CA:

Overall probability: 0.360

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU81	0.00	1.00
LEU82	0.51	1.00
GLN83	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L81HA	1.00
L82HB2	1.00
L82HB3	1.00
L82HG	1.00
L82HD11	0.99
L82HD21	0.99
L82H	1.00
L82HA	1.00
Q83HA	1.00
Q83H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU81	HA	1.00	0.048	0.00	0.00
LEU82	HA	1.00	0.007	1.00	3.01
LEU82	HB2	1.00	0.043	0.00	0.00
LEU82	HB3	1.00	0.028	1.00	0.39
LEU82	HG	1.00	0.066	0.00	0.00
LEU82	HD11	0.99	0.034	0.60	0.00
LEU82	HD21	0.99	0.013	1.00	1.41
LEU82	H	1.00	0.120	0.00	0.00
GLN83	HA	1.00	0.057	0.00	0.00
GLN83	H	1.00	0.129	0.00	0.00

3.82.2 Detailed Probabilities of LEU82CB:

Overall probability: 0.838

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU82	0.96	1.00
GLN83	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L82HA	1.00
L82HB3	1.00
L82HG	1.00
L82HD11	1.00
L82HD21	1.00
L82H	1.00
L82HB2	1.00
Q83H	1.00

NOESY contacts detailed probability

3.82 LEU(82)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU82	HA	1.00	0.002	1.00	0.19
LEU82	HB2	1.00	0.003	1.00	1.46
LEU82	HB3	1.00	0.001	1.00	0.79
LEU82	HG	1.00	0.020	1.00	1.46
LEU82	HD11	1.00	0.014	1.00	0.68
LEU82	HD21	1.00	0.033	0.70	0.00
LEU82	H	1.00	0.008	1.00	0.18
GLN83	H	1.00	0.435	0.00	0.00

3.82.3 Detailed Probabilities of LEU82CG:

Overall probability: 0.777

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU82	0.89	1.00
GLN83	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
L82HA	1.00
L82HB2	1.00
L82HB3	1.00
L82HD11	1.00
L82HD21	1.00
L82H	1.00
L82HG	1.00
Q83H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU82	HA	1.00	0.008	1.00	0.09
LEU82	HB2	1.00	0.015	1.00	19.97
LEU82	HB3	1.00	0.029	1.00	2.53
LEU82	HG	1.00	0.038	0.20	0.00
LEU82	HD11	1.00	0.018	1.00	2.48
LEU82	HD21	1.00	0.029	1.00	2.48
LEU82	H	1.00	0.005	1.00	0.15
GLN83	H	0.98	0.104	0.02	0.00

3.82.4 Detailed Probabilities of LEU82CD1:

Overall probability: 0.001

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU82	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L82HA	0.99
L82HB2	1.00
L82HB3	1.00
L82HG	1.00
L82HD12	1.00
L82HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU82	HA	0.99	0.103	0.01	0.00
LEU82	HB2	1.00	0.563	0.00	0.00
LEU82	HB3	1.00	0.448	0.00	0.00
LEU82	HG	1.00	0.586	0.00	0.00
LEU82	HD11	1.00	0.596	0.00	0.00
LEU82	HD21	1.00	0.643	0.00	0.00

3.82.5 Detailed Probabilities of LEU82CD2:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU82	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
L82HA	0.99
L82HB2	1.00
L82HB3	1.00
L82HG	1.00
L82HD11	1.00
L82HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU82	HA	0.99	0.003	1.00	1.01
LEU82	HB2	1.00	0.127	0.00	0.00
LEU82	HB3	1.00	0.012	1.00	0.73
LEU82	HG	1.00	0.150	0.00	0.00
LEU82	HD11	1.00	0.056	0.00	0.00
LEU82	HD21	1.00	0.009	1.00	44.16

3.82.6 Detailed Probabilities of LEU82N:

Overall probability: 0.929

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU81	0.83	1.00
LEU82	1.00	1.00
GLN83	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L81HB3	1.00
L81HB2	1.00
L81HA	1.00
L81H	1.00
L81HG	0.98
L82HA	1.00
L82HB2	1.00
L82HB3	1.00
L82HG	1.00
L82H	1.00
Q83H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU81	HA	1.00	0.001	1.00	-1621019.00
LEU81	HB2	1.00	0.004	1.00	-134613.00
LEU81	HB3	1.00	0.005	1.00	-399450.00
LEU81	HG	0.98	0.005	1.00	-399450.00
LEU81	H	1.00	0.087	0.00	0.00
LEU81	HD11	0.53	0.001	1.00	-1194892.00
LEU82	HA	1.00	0.004	1.00	-276539.00
LEU82	HB2	1.00	0.010	1.00	-738603.00
LEU82	HB3	1.00	0.003	1.00	-655429.00
LEU82	HG	1.00	0.013	1.00	-738603.00
LEU82	H	1.00	0.004	1.00	-4019906.00
LEU82	HD11	0.88	0.010	1.00	-1194892.00
GLN83	H	1.00	0.005	1.00	-104325.00
GLN83	HA	0.92	0.008	1.00	-1621019.00

3.82.7 Detailed Probabilities of LEU82HA:

Overall probability: 0.701

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU81	1.00	1.00
LEU82	0.72	1.00
GLN83	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
L81HA	1.00
L82HB2	1.00
L82HB3	1.00
L82HG	1.00
L82HD11	0.99
L82HD21	0.99
L82H	1.00
L82HA	1.00
Q83HA	1.00
Q83H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU81	HA	1.00	0.000	1.00	0.11
LEU82	HA	1.00	0.007	1.00	3.01
LEU82	HB2	1.00	0.002	1.00	0.19
LEU82	HB3	1.00	1.775	0.00	0.00
LEU82	HG	1.00	0.008	1.00	0.09
LEU82	HD11	0.99	0.103	0.01	0.00
LEU82	HD21	0.99	0.003	1.00	1.01
LEU82	H	1.00	0.004	1.00	-276539.00
GLN83	HA	1.00	0.351	0.00	0.00
GLN83	H	1.00	0.002	1.00	-1721778.00

3.82.8 Detailed Probabilities of LEU82HB2:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU82	0.43	1.00
GLN83	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L82HA	1.00
L82HB3	1.00
L82HG	1.00
L82HD11	1.00
L82HD21	1.00
L82H	1.00
L82HB2	1.00
Q83H	1.00

NOESY contacts detailed probability

3.82 LEU(82)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU82	HA	1.00	0.043	0.00	0.00
LEU82	HB2	1.00	0.003	1.00	1.46
LEU82	HB3	1.00	0.129	0.00	0.00
LEU82	HG	1.00	0.015	1.00	19.97
LEU82	HD11	1.00	0.563	0.00	0.00
LEU82	HD21	1.00	0.127	0.00	0.00
LEU82	H	1.00	0.010	1.00	-738603.00
GLN83	H	1.00	0.004	1.00	-419587.00

3.82.9 Detailed Probabilities of LEU82HB3:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU82	0.71	1.00
GLN83	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L82HA	1.00
L82HB2	1.00
L82HG	1.00
L82HD11	1.00
L82HD21	1.00
L82H	1.00
L82HB3	1.00
Q83H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU82	HA	1.00	0.028	1.00	0.39
LEU82	HB2	1.00	0.001	1.00	0.79
LEU82	HB3	1.00	0.113	0.00	0.00
LEU82	HG	1.00	0.029	1.00	2.53
LEU82	HD11	1.00	0.448	0.00	0.00
LEU82	HD21	1.00	0.012	1.00	0.73
LEU82	H	1.00	0.003	1.00	-655429.00
GLN83	H	1.00	0.001	1.00	-255852.00

3.82.10 Detailed Probabilities of LEU82HG:

Overall probability: 0.400

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU82	0.31	1.00
GLN83	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L82HA	1.00
L82HB2	1.00
L82HB3	1.00
L82HD11	1.00
L82HD21	1.00
L82H	1.00
L82HG	1.00
Q83H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU82	HA	1.00	0.066	0.00	0.00
LEU82	HB2	1.00	0.020	1.00	1.46
LEU82	HB3	1.00	0.106	0.00	0.00
LEU82	HG	1.00	0.038	0.20	0.00
LEU82	HD11	1.00	0.586	0.00	0.00
LEU82	HD21	1.00	0.150	0.00	0.00
LEU82	H	1.00	0.013	1.00	-738603.00
GLN83	H	0.98	0.019	1.00	-419587.00

3.82.11 Detailed Probabilities of LEU82HD11:

Overall probability: 0.657

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU82	0.66	1.00

Expected NOESY Contacts

Proton	Expected probability
L82HA	0.99
L82HB2	1.00
L82HB3	1.00
L82HG	1.00
L82HD12	1.00
L82HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU82	HA	0.99	0.034	0.60	0.00
LEU82	HB2	1.00	0.014	1.00	0.68
LEU82	HB3	1.00	0.010	1.00	0.53
LEU82	HG	1.00	0.018	1.00	2.48
LEU82	HD11	1.00	0.596	0.00	0.00
LEU82	HD21	1.00	0.056	0.00	0.00
LEU82	H	0.86	0.010	1.00	-1194892.00

3.82.12 Detailed Probabilities of LEU82HD21:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU82	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
L82HA	0.99
L82HB2	1.00
L82HB3	1.00
L82HG	1.00
L82HD11	1.00
L82HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU82	HA	0.99	0.013	1.00	1.41
LEU82	HB2	1.00	0.033	0.70	0.00
LEU82	HB3	1.00	0.037	0.30	0.00
LEU82	HG	1.00	0.029	1.00	2.48
LEU82	HD11	1.00	0.643	0.00	0.00
LEU82	HD21	1.00	0.009	1.00	44.16

3.82.13 Detailed Probabilities of LEU82H:

Overall probability: 0.923

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU81	1.00	1.00
LEU82	0.80	1.00
GLN83	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L81HB3	1.00
L81HB2	1.00
L81HA	1.00
L81H	1.00
L81HG	0.98
L82HA	1.00
L82HB2	1.00
L82HB3	1.00
L82HG	1.00
L82H	1.00
Q83H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU81	HA	1.00	0.005	1.00	0.88
LEU81	HB2	1.00	0.009	1.00	0.06
LEU81	HB3	1.00	0.005	1.00	0.06
LEU81	HG	0.98	0.006	1.00	0.18
LEU81	H	1.00	0.013	1.00	-118622.00
LEU81	HD11	0.53	0.001	1.00	0.77
LEU82	HA	1.00	0.120	0.00	0.00
LEU82	HB2	1.00	0.008	1.00	0.18
LEU82	HB3	1.00	0.003	1.00	0.18
LEU82	HG	1.00	0.005	1.00	0.15
LEU82	H	1.00	0.004	1.00	-4019906.00
GLN83	H	1.00	0.010	1.00	-120255.00
GLN83	HA	0.92	0.009	1.00	0.06

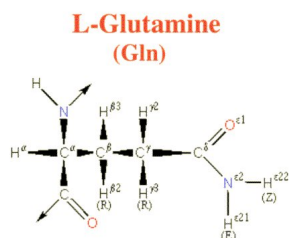


Figure 82: Image from the BMRB

Residue probability: 0.865
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.333	176.405	1.998	0.000	0.000
CA 3.83.1	54.586	56.667	2.318	0.727	1.000
CB 3.83.2	29.870	29.436	2.799	1.000	1.000
CG 3.83.3	33.720	33.781	1.871	0.889	1.000
N 3.83.4	122.153	119.799	3.762	0.992	1.000
NE2 3.83.5	110.447	111.924	2.434	1.000	1.000
HA 3.83.6	5.260	4.265	0.455	0.909	1.000
HB2 3.83.7	2.212	2.047	0.290	0.800	1.000
HB3 3.83.8	1.420	2.012	0.313	1.000	1.000
HG2 3.83.9	2.336	2.308	0.289	0.656	1.000
HG3 3.83.10	2.117	2.284	0.313	0.889	1.000
H 3.83.11	8.437	8.232	0.711	0.668	1.000
HE21 3.83.12	7.201	7.217	0.496	0.857	1.000
HE22 3.83.13	7.200	7.041	0.463	0.857	1.000

3.83.1 Detailed Probabilities of GLN83CA:

Overall probability: 0.727
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU82	0.50	1.00
GLN83	0.86	1.00
ASP84	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
L82HA	1.00
Q83HB2	1.00
Q83HB3	1.00
Q83HG2	1.00
Q83HG3	1.00
Q83H	1.00
Q83HA	1.00
D84H	1.00
D84HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU82	HA	1.00	0.351	0.00	0.00
LEU82	H	0.92	0.009	1.00	0.06
GLN83	HA	1.00	0.002	1.00	2.16
GLN83	HB2	1.00	0.005	1.00	0.20
GLN83	HB3	1.00	0.006	1.00	0.33
GLN83	HG2	1.00	0.119	0.00	0.00
GLN83	HG3	1.00	0.013	1.00	0.31
GLN83	H	1.00	0.004	1.00	0.26
GLN83	HE21	0.94	0.023	1.00	0.08
ASP84	HA	1.00	0.169	0.00	0.00
ASP84	H	1.00	0.004	1.00	0.72

3.83.2 Detailed Probabilities of GLN83CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN83	1.00	1.00
ASP84	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q83HA	1.00
Q83HB2	1.00
Q83HG2	1.00
Q83HG3	1.00
Q83H	1.00
Q83HE21	1.00
Q83HE22	1.00
Q83HB3	1.00
D84H	1.00

NOESY contacts detailed probability

3.83 GLN(83)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN83	HA	1.00	0.007	1.00	0.25
GLN83	HB2	1.00	0.004	1.00	0.83
GLN83	HB3	1.00	0.011	1.00	0.99
GLN83	HG2	1.00	0.002	1.00	0.30
GLN83	HG3	1.00	0.007	1.00	0.43
GLN83	H	1.00	0.005	1.00	0.18
GLN83	HE21	1.00	0.023	1.00	0.07
GLN83	HE22	1.00	0.024	1.00	0.07
ASP84	H	1.00	0.015	1.00	0.05

3.83.3 Detailed Probabilities of GLN83CG:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN83	0.88	1.00
ASP84	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q83HA	1.00
Q83HB2	1.00
Q83HB3	1.00
Q83HG2	1.00
Q83H	1.00
Q83HE21	1.00
Q83HE22	1.00
Q83HG3	1.00
D84H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN83	HA	1.00	0.002	1.00	0.20
GLN83	HB2	1.00	0.087	0.00	0.00
GLN83	HB3	1.00	0.006	1.00	0.47
GLN83	HG2	1.00	0.001	1.00	1.80
GLN83	HG3	1.00	0.001	1.00	3.35
GLN83	H	1.00	0.000	1.00	0.11
GLN83	HE21	1.00	0.005	1.00	0.37
GLN83	HE22	1.00	0.006	1.00	0.37
ASP84	H	0.96	0.012	1.00	0.10

3.83.4 Detailed Probabilities of GLN83N:

Overall probability: 0.992

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU82	1.00	1.00
GLN83	0.98	1.00
ASP84	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L82H	1.00
L82HB3	1.00
L82HB2	1.00
L82HA	1.00
L82HG	0.98
Q83HA	1.00
Q83HB2	1.00
Q83HB3	1.00
Q83HG2	1.00
Q83HG3	1.00
Q83H	1.00
D84H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU82	HA	1.00	0.002	1.00	-1721778.00
LEU82	HB2	1.00	0.004	1.00	-419587.00
LEU82	HB3	1.00	0.001	1.00	-255852.00
LEU82	HG	0.98	0.019	1.00	-419587.00
LEU82	H	1.00	0.010	1.00	-120255.00
LEU82	HD21	0.58	0.013	1.00	-649406.00
GLN83	HA	1.00	0.004	1.00	-457948.00
GLN83	HB2	1.00	0.008	1.00	-557367.00
GLN83	HB3	1.00	0.007	1.00	-519520.00
GLN83	HG2	1.00	0.031	0.90	0.00
GLN83	HG3	1.00	0.018	1.00	-203902.00
GLN83	H	1.00	0.001	1.00	-7675379.00
ASP84	H	1.00	0.004	1.00	-148676.00

3.83.5 Detailed Probabilities of GLN83NE2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN83	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q83HB2	1.00
Q83HB3	1.00
Q83HG2	1.00
Q83HG3	1.00
Q83HE22	1.00
Q83HE21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN83	HB2	1.00	0.014	1.00	-159812.00
GLN83	HB3	1.00	0.005	1.00	-201185.00
GLN83	HG2	1.00	0.002	1.00	-652972.00
GLN83	HG3	1.00	0.002	1.00	-512020.00
GLN83	HE21	1.00	0.002	1.00	-12590931.00
GLN83	HE22	1.00	0.003	1.00	-12590931.00
GLN83	HA	0.94	0.003	1.00	-96745.00

3.83.6 Detailed Probabilities of GLN83HA:

Overall probability: 0.909

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU82	0.50	1.00
GLN83	1.00	1.00
ASP84	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L82HA	1.00
Q83HB2	1.00
Q83HB3	1.00
Q83HG2	1.00
Q83HG3	1.00
Q83H	1.00
Q83HA	1.00
D84H	1.00
D84HA	1.00

NOESY contacts detailed probability

3.83 GLN(83)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU82	HA	1.00	0.057	0.00	0.00
LEU82	H	0.92	0.008	1.00	-1621019.00
GLN83	HA	1.00	0.002	1.00	2.16
GLN83	HB2	1.00	0.004	1.00	0.22
GLN83	HB3	1.00	0.007	1.00	0.25
GLN83	HG2	1.00	0.001	1.00	0.23
GLN83	HG3	1.00	0.002	1.00	0.20
GLN83	H	1.00	0.004	1.00	-457948.00
GLN83	HE21	0.94	0.003	1.00	-96745.00
ASP84	HA	1.00	0.017	1.00	0.05
ASP84	H	1.00	0.000	1.00	-1120541.00

3.83.7 Detailed Probabilities of GLN83HB2:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN83	0.75	1.00
ASP84	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q83HA	1.00
Q83HB3	1.00
Q83HG2	1.00
Q83HG3	1.00
Q83H	1.00
Q83HE21	1.00
Q83HE22	1.00
Q83HB2	1.00
D84H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN83	HA	1.00	0.005	1.00	0.20
GLN83	HB2	1.00	0.030	1.00	0.00
GLN83	HB3	1.00	0.004	1.00	0.83
GLN83	HG2	1.00	0.095	0.00	0.00
GLN83	HG3	1.00	0.087	0.00	0.00
GLN83	H	1.00	0.008	1.00	-557367.00
GLN83	HE21	1.00	0.014	1.00	-159812.00
GLN83	HE22	1.00	0.014	1.00	-159812.00
ASP84	H	1.00	0.008	1.00	-113172.00
ASP84	HA	0.61	0.024	1.00	0.51

3.83.8 Detailed Probabilities of GLN83HB3:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN83	1.00	1.00
ASP84	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q83HA	1.00
Q83HB2	1.00
Q83HG2	1.00
Q83HG3	1.00
Q83H	1.00
Q83HE21	1.00
Q83HE22	1.00
Q83HB3	1.00
D84H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN83	HA	1.00	0.006	1.00	0.33
GLN83	HB2	1.00	0.008	1.00	0.87
GLN83	HB3	1.00	0.011	1.00	0.99
GLN83	HG2	1.00	0.004	1.00	0.40
GLN83	HG3	1.00	0.006	1.00	0.47
GLN83	H	1.00	0.007	1.00	-519520.00
GLN83	HE21	1.00	0.005	1.00	-201185.00
GLN83	HE22	1.00	0.005	1.00	-201185.00
ASP84	H	1.00	0.008	1.00	-182051.00

3.83.9 Detailed Probabilities of GLN83HG2:

Overall probability: 0.656

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN83	0.61	1.00
ASP84	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q83HA	1.00
Q83HB2	1.00
Q83HB3	1.00
Q83HG3	1.00
Q83H	1.00
Q83HE21	1.00
Q83HE22	1.00
Q83HG2	1.00
D84H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN83	HA	1.00	0.119	0.00	0.00
GLN83	HB2	1.00	0.077	0.00	0.00
GLN83	HB3	1.00	0.002	1.00	0.30
GLN83	HG2	1.00	0.219	0.00	0.00
GLN83	HG3	1.00	0.001	1.00	1.80
GLN83	H	1.00	0.031	0.90	0.00
GLN83	HE21	1.00	0.002	1.00	-652972.00
GLN83	HE22	1.00	0.002	1.00	-652972.00
ASP84	H	0.98	0.002	1.00	-312887.00

3.83.10 Detailed Probabilities of GLN83HG3:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN83	0.88	1.00
ASP84	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q83HA	1.00
Q83HB2	1.00
Q83HB3	1.00
Q83HG2	1.00
Q83H	1.00
Q83HE21	1.00
Q83HE22	1.00
Q83HG3	1.00
D84H	0.96

NOESY contacts detailed probability

3.83 GLN(83)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN83	HA	1.00	0.013	1.00	0.31
GLN83	HB2	1.00	0.065	0.00	0.00
GLN83	HB3	1.00	0.007	1.00	0.43
GLN83	HG2	1.00	0.000	1.00	1.55
GLN83	HG3	1.00	0.001	1.00	3.35
GLN83	H	1.00	0.018	1.00	-203902.00
GLN83	HE21	1.00	0.002	1.00	-512020.00
GLN83	HE22	1.00	0.002	1.00	-512020.00
ASP84	H	0.96	0.005	1.00	-252310.00

3.83.11 Detailed Probabilities of GLN83H:

Overall probability: 0.668

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU82	0.40	1.00
GLN83	0.83	1.00
ASP84	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L82H	1.00
L82HB3	1.00
L82HB2	1.00
L82HA	1.00
L82HG	0.98
Q83HA	1.00
Q83HB2	1.00
Q83HB3	1.00
Q83HG2	1.00
Q83HG3	1.00
Q83H	1.00
D84H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU82	HA	1.00	0.129	0.00	0.00
LEU82	HB2	1.00	0.435	0.00	0.00
LEU82	HB3	1.00	0.005	1.00	0.07
LEU82	HG	0.98	0.104	0.02	0.00
LEU82	H	1.00	0.005	1.00	-104325.00
GLN83	HA	1.00	0.004	1.00	0.26
GLN83	HB2	1.00	0.123	0.00	0.00
GLN83	HB3	1.00	0.005	1.00	0.18
GLN83	HG2	1.00	0.008	1.00	0.05
GLN83	HG3	1.00	0.000	1.00	0.11
GLN83	H	1.00	0.001	1.00	-7675379.00
ASP84	H	1.00	0.003	1.00	-157374.00

3.83.12 Detailed Probabilities of GLN83HE21:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN83	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
Q83HB2	1.00
Q83HB3	1.00
Q83HG2	1.00
Q83HG3	1.00
Q83HE22	1.00
Q83HE21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN83	HB2	1.00	0.216	0.00	0.00
GLN83	HB3	1.00	0.024	1.00	0.07
GLN83	HG2	1.00	0.008	1.00	0.40
GLN83	HG3	1.00	0.006	1.00	0.37
GLN83	HE21	1.00	0.003	1.00	-12590931.00
GLN83	HE22	1.00	0.003	1.00	-12590931.00
GLN83	HA	0.94	0.023	1.00	0.08

3.83.13 Detailed Probabilities of GLN83HE22:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN83	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
Q83HB2	1.00
Q83HB3	1.00
Q83HG2	1.00
Q83HG3	1.00
Q83HE21	1.00
Q83HE22	1.00

NOESY contacts detailed probability

3.83 GLN(83)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN83	HB2	1.00	0.216	0.00	0.00
GLN83	HB3	1.00	0.024	1.00	0.07
GLN83	HG2	1.00	0.008	1.00	0.40
GLN83	HG3	1.00	0.006	1.00	0.37
GLN83	HE21	1.00	0.003	1.00	-12590931.00
GLN83	HE22	1.00	0.003	1.00	-12590931.00
GLN83	HA	0.94	0.023	1.00	0.08

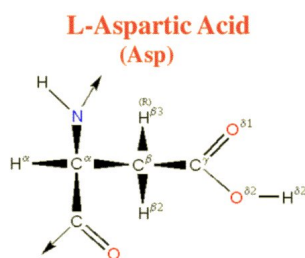
3.84 ASP(84)

Figure 83: Image from the BMRB

Residue probability: 0.893

Residue probability confidence: 0.893

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.308	176.463	2.348	0.000	0.000
CA 3.84.1	54.015	54.786	4.266	0.875	0.875
CB 3.84.2	43.771	40.949	3.070	1.000	0.833
N 3.84.3	124.451	120.550	5.690	1.000	1.000
HD2	NA	—	—	0.000	0.000
HA 3.84.4	4.502	4.587	0.329	0.857	0.875
HB2 3.84.5	2.588	2.708	0.282	0.600	0.833
HB3 3.84.6	2.664	2.654	0.285	1.000	0.833
H 3.84.7	8.205	8.304	1.027	0.917	1.000

3.84.1 Detailed Probabilities of ASP84CA:

Overall probability: 0.875

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN83	1.00	1.00
ASP84	0.75	0.80
GLN85	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q83HA	1.00
D84HD2	1.00
D84HB2	1.00
D84HB3	1.00
D84H	1.00
D84HA	1.00
Q85H	1.00
Q85HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN83	HA	1.00	0.017	1.00	0.05
GLN83	HB2	0.61	0.024	1.00	0.51
ASP84	HA	1.00	0.000	1.00	10.31
ASP84	HB2	1.00	0.071	0.00	0.00
ASP84	HB3	1.00	0.005	1.00	0.77
ASP84	H	1.00	0.006	1.00	0.51
GLN85	HA	1.00	0.001	1.00	0.13
GLN85	H	1.00	0.008	1.00	1.50

3.84.2 Detailed Probabilities of ASP84CB:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP84	1.00	0.80
GLN85	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D84HD2	1.00
D84HA	1.00
D84HB3	1.00
D84H	1.00
D84HB2	1.00
Q85H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP84	HA	1.00	0.002	1.00	0.38
ASP84	HB2	1.00	0.005	1.00	2.41
ASP84	HB3	1.00	0.002	1.00	1.94
ASP84	H	1.00	0.007	1.00	0.17
GLN85	H	1.00	0.013	1.00	0.11

3.84.3 Detailed Probabilities of ASP84N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN83	1.00	1.00
ASP84	1.00	1.00
GLN85	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q83HB3	1.00
Q83HB2	1.00
Q83H	1.00
Q83HG2	0.98
Q83HA	1.00
Q83HG3	0.96
D84HA	1.00
D84HB2	1.00
D84HB3	1.00
D84H	1.00
Q85H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN83	HA	1.00	0.000	1.00	-1120541.00
GLN83	HB2	1.00	0.008	1.00	-113172.00
GLN83	HB3	1.00	0.008	1.00	-182051.00
GLN83	HG2	0.98	0.002	1.00	-312887.00
GLN83	HG3	0.96	0.005	1.00	-252310.00
GLN83	H	1.00	0.003	1.00	-157374.00
ASP84	HA	1.00	0.001	1.00	-496670.00
ASP84	HB2	1.00	0.007	1.00	-265898.00
ASP84	HB3	1.00	0.005	1.00	-260588.00
ASP84	H	1.00	0.004	1.00	-3576824.00
GLN85	H	1.00	0.019	1.00	-160863.00
GLN85	HA	0.84	0.010	1.00	-78401.00

3.84.4 Detailed Probabilities of ASP84HA:

Overall probability: 0.857

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN83	0.00	1.00
ASP84	1.00	0.80
GLN85	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q83HA	1.00
D84HD2	1.00
D84HB2	1.00
D84HB3	1.00
D84H	1.00
D84HA	1.00
Q85H	1.00
Q85HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN83	HA	1.00	0.169	0.00	0.00
ASP84	HA	1.00	0.000	1.00	10.31
ASP84	HB2	1.00	0.002	1.00	0.38
ASP84	HB3	1.00	0.002	1.00	0.44
ASP84	H	1.00	0.001	1.00	-496670.00
GLN85	HA	1.00	0.005	1.00	0.38
GLN85	H	1.00	0.000	1.00	-1784708.00

3.84.5 Detailed Probabilities of ASP84HB2:

Overall probability: 0.600

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP84	0.50	0.80
GLN85	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D84HD2	1.00
D84HA	1.00
D84HB3	1.00
D84H	1.00
D84HB2	1.00
Q85H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP84	HA	1.00	0.071	0.00	0.00
ASP84	HB2	1.00	0.005	1.00	2.41
ASP84	HB3	1.00	0.070	0.00	0.00
ASP84	H	1.00	0.007	1.00	-265898.00
GLN85	H	1.00	0.002	1.00	-247489.00

3.84.6 Detailed Probabilities of ASP84HB3:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP84	1.00	0.80
GLN85	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D84HD2	1.00
D84HA	1.00
D84HB2	1.00
D84H	1.00
D84HB3	1.00
Q85H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP84	HA	1.00	0.005	1.00	0.77
ASP84	HB2	1.00	0.002	1.00	1.94
ASP84	HB3	1.00	0.006	1.00	2.32
ASP84	H	1.00	0.005	1.00	-260588.00
GLN85	H	1.00	0.020	1.00	-247077.00

3.84.7 Detailed Probabilities of ASP84H:

Overall probability: 0.917

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN83	0.83	1.00
ASP84	1.00	1.00
GLN85	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q83HB3	1.00
Q83HB2	1.00
Q83H	1.00
Q83HG2	0.98
Q83HA	1.00
Q83HG3	0.96
D84HA	1.00
D84HB2	1.00
D84HB3	1.00
D84H	1.00
Q85H	1.00

NOESY contacts detailed probability

3.84 ASP(84)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN83	HA	1.00	0.004	1.00	0.72
GLN83	HB2	1.00	0.109	0.00	0.00
GLN83	HB3	1.00	0.015	1.00	0.05
GLN83	HG2	0.98	0.004	1.00	0.17
GLN83	HG3	0.96	0.012	1.00	0.10
GLN83	H	1.00	0.004	1.00	-148676.00
ASP84	HA	1.00	0.006	1.00	0.51
ASP84	HB2	1.00	0.007	1.00	0.17
ASP84	HB3	1.00	0.011	1.00	0.18
ASP84	H	1.00	0.004	1.00	-3576824.00
GLN85	H	1.00	0.006	1.00	-154975.00
GLN85	HA	0.84	0.014	1.00	0.08

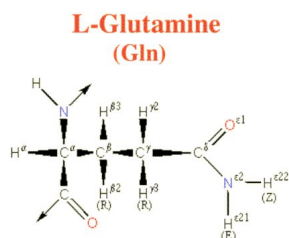


Figure 84: Image from the BMRB

Residue probability: 0.851
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	175.431	176.405	1.998	0.000	0.000
CA 3.85.1	56.595	56.667	2.318	0.800	1.000
CB 3.85.2	29.334	29.436	2.799	0.889	1.000
CG 3.85.3	33.720	33.781	1.871	0.782	1.000
N 3.85.4	120.202	119.799	3.762	0.917	1.000
NE2 3.85.5	112.150	111.924	2.434	1.000	1.000
HA 3.85.6	4.334	4.265	0.455	0.750	1.000
HB2 3.85.7	2.173	2.047	0.290	0.900	1.000
HB3 3.85.8	2.040	2.012	0.313	0.889	1.000
HG2 3.85.9	2.407	2.308	0.289	0.778	1.000
HG3 3.85.10	2.405	2.284	0.313	0.778	1.000
H 3.85.11	8.617	8.232	0.711	0.818	1.000
HE21 3.85.12	7.624	7.217	0.496	0.933	1.000
HE22 3.85.13	6.895	7.041	0.463	0.833	1.000

3.85.1 Detailed Probabilities of GLN85CA:

Overall probability: 0.800
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP84	1.00	1.00
GLN85	1.00	1.00
ASP86	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D84HA	1.00
Q85HB2	1.00
Q85HB3	1.00
Q85HG2	1.00
Q85HG3	1.00
Q85H	1.00
Q85HA	1.00
D86H	1.00
D86HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP84	HA	1.00	0.005	1.00	0.38
ASP84	H	0.84	0.014	1.00	0.08
GLN85	HA	1.00	0.024	1.00	21.81
GLN85	HB2	1.00	0.006	1.00	1.16
GLN85	HB3	1.00	0.000	1.00	1.02
GLN85	HG2	1.00	0.001	1.00	0.65
GLN85	HG3	1.00	0.003	1.00	0.65
GLN85	H	1.00	0.013	1.00	0.57
ASP86	HA	1.00	0.074	0.00	0.00
ASP86	H	1.00	0.061	0.00	0.00

3.85.2 Detailed Probabilities of GLN85CB:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN85	0.88	1.00
ASP86	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q85HA	1.00
Q85HB3	1.00
Q85HG2	1.00
Q85HG3	1.00
Q85H	1.00
Q85HE21	1.00
Q85HE22	1.00
Q85HB2	1.00
D86H	1.00

NOESY contacts detailed probability

3.85 GLN(85)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN85	HA	1.00	0.005	1.00	1.86
GLN85	HB2	1.00	0.009	1.00	19.33
GLN85	HB3	1.00	0.016	1.00	12.14
GLN85	HG2	1.00	0.006	1.00	2.85
GLN85	HG3	1.00	0.008	1.00	2.85
GLN85	H	1.00	0.051	0.00	0.00
GLN85	HE21	1.00	0.008	1.00	0.92
GLN85	HE22	1.00	0.022	1.00	0.06
ASP86	H	1.00	0.023	1.00	0.79

3.85.3 Detailed Probabilities of GLN85CG:

Overall probability: 0.782

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN85	0.88	1.00
ASP86	0.04	1.00

Expected NOESY Contacts

Proton	Expected probability
Q85HA	1.00
Q85HB2	1.00
Q85HB3	1.00
Q85HG2	1.00
Q85H	1.00
Q85HE21	1.00
Q85HE22	1.00
Q85HG3	1.00
D86H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN85	HA	1.00	0.115	0.00	0.00
GLN85	HB2	1.00	0.017	1.00	4.31
GLN85	HB3	1.00	0.000	1.00	2.35
GLN85	HG2	1.00	0.009	1.00	103.18
GLN85	HG3	1.00	0.011	1.00	103.18
GLN85	H	1.00	0.011	1.00	0.69
GLN85	HE21	1.00	0.009	1.00	0.76
GLN85	HE22	1.00	0.001	1.00	0.45
ASP86	H	0.96	0.063	0.04	0.00

3.85.4 Detailed Probabilities of GLN85N:

Overall probability: 0.917

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP84	1.00	1.00
GLN85	1.00	1.00
ASP86	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
D84HA	1.00
D84H	1.00
D84HB2	1.00
D84HB3	1.00
Q85HA	1.00
Q85HB2	1.00
Q85HB3	1.00
Q85HG2	1.00
Q85HG3	1.00
Q85H	1.00
D86H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP84	HA	1.00	0.000	1.00	-1784708.00
ASP84	HB2	1.00	0.002	1.00	-247489.00
ASP84	HB3	1.00	0.020	1.00	-247077.00
ASP84	H	1.00	0.006	1.00	-154975.00
GLN85	HA	1.00	0.012	1.00	-648935.00
GLN85	HB2	1.00	0.006	1.00	-573044.00
GLN85	HB3	1.00	0.002	1.00	-943048.00
GLN85	HG2	1.00	0.003	1.00	-594625.00
GLN85	HG3	1.00	0.005	1.00	-594625.00
GLN85	H	1.00	0.005	1.00	-5727664.00
ASP86	H	1.00	0.069	0.00	0.00
ASP86	HA	0.86	0.001	1.00	-73717.00

3.85.5 Detailed Probabilities of GLN85NE2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN85	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q85HB2	1.00
Q85HB3	1.00
Q85HG2	1.00
Q85HG3	1.00
Q85HE22	1.00
Q85HE21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN85	HB2	1.00	0.010	1.00	-126014.00
GLN85	HB3	1.00	0.000	1.00	-109753.00
GLN85	HG2	1.00	0.004	1.00	-1060125.00
GLN85	HG3	1.00	0.006	1.00	-1060125.00
GLN85	HE21	1.00	0.000	1.00	-33873372.00
GLN85	HE22	1.00	0.001	1.00	-14559339.00
GLN85	HA	0.94	0.011	1.00	-75502.00

3.85.6 Detailed Probabilities of GLN85HA:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP84	1.00	1.00
GLN85	0.71	1.00
ASP86	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
D84HA	1.00
Q85HB2	1.00
Q85HB3	1.00
Q85HG2	1.00
Q85HG3	1.00
Q85H	1.00
Q85HA	1.00
D86H	1.00
D86HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP84	HA	1.00	0.001	1.00	0.13
ASP84	HB3	0.84	0.006	1.00	0.07
ASP84	H	0.84	0.010	1.00	-78401.00
GLN85	HA	1.00	0.024	1.00	21.81
GLN85	HB2	1.00	0.005	1.00	1.86
GLN85	HB3	1.00	0.001	1.00	0.59
GLN85	HG2	1.00	0.115	0.00	0.00
GLN85	HG3	1.00	0.115	0.00	0.00
GLN85	H	1.00	0.012	1.00	-648935.00
GLN85	HE21	0.94	0.011	1.00	-75502.00
ASP86	HA	1.00	0.057	0.00	0.00
ASP86	H	1.00	0.012	1.00	-712495.00

3.85.7 Detailed Probabilities of GLN85HB2:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN85	0.88	1.00
ASP86	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q85HA	1.00
Q85HB3	1.00
Q85HG2	1.00
Q85HG3	1.00
Q85H	1.00
Q85HE21	1.00
Q85HE22	1.00
Q85HB2	1.00
D86H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN85	HA	1.00	0.006	1.00	1.16
GLN85	HB2	1.00	0.009	1.00	19.33
GLN85	HB3	1.00	0.009	1.00	14.03
GLN85	HG2	1.00	0.017	1.00	4.31
GLN85	HG3	1.00	0.017	1.00	4.31
GLN85	H	1.00	0.006	1.00	-573044.00
GLN85	HE21	1.00	0.010	1.00	-126014.00
GLN85	HE22	1.00	1.357	0.00	0.00
ASP86	H	1.00	0.008	1.00	-296128.00
ASP86	HA	0.61	0.023	1.00	0.50

3.85.8 Detailed Probabilities of GLN85HB3:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN85	0.88	1.00
ASP86	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q85HA	1.00
Q85HB2	1.00
Q85HG2	1.00
Q85HG3	1.00
Q85H	1.00
Q85HE21	1.00
Q85HE22	1.00
Q85HB3	1.00
D86H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN85	HA	1.00	0.000	1.00	1.02
GLN85	HB2	1.00	0.016	1.00	12.14
GLN85	HB3	1.00	0.001	1.00	52.03
GLN85	HG2	1.00	0.000	1.00	2.35
GLN85	HG3	1.00	0.000	1.00	2.35
GLN85	H	1.00	0.002	1.00	-943048.00
GLN85	HE21	1.00	0.000	1.00	-109753.00
GLN85	HE22	1.00	1.224	0.00	0.00
ASP86	H	1.00	0.004	1.00	-460067.00

3.85.9 Detailed Probabilities of GLN85HG2:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN85	0.75	1.00
ASP86	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q85HA	1.00
Q85HB2	1.00
Q85HB3	1.00
Q85HG3	1.00
Q85H	1.00
Q85HE21	1.00
Q85HE22	1.00
Q85HG2	1.00
D86H	0.98

NOESY contacts detailed probability

3.85 GLN(85)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN85	HA	1.00	0.001	1.00	0.65
GLN85	HB2	1.00	0.006	1.00	2.85
GLN85	HB3	1.00	0.072	0.00	0.00
GLN85	HG2	1.00	0.009	1.00	103.18
GLN85	HG3	1.00	0.009	1.00	103.18
GLN85	H	1.00	0.003	1.00	-594625.00
GLN85	HE21	1.00	0.004	1.00	-1060125.00
GLN85	HE22	1.00	1.591	0.00	0.00
ASP86	H	0.98	0.003	1.00	-238011.00

3.85.10 Detailed Probabilities of GLN85HG3:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN85	0.75	1.00
ASP86	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q85HA	1.00
Q85HB2	1.00
Q85HB3	1.00
Q85HG2	1.00
Q85H	1.00
Q85HE21	1.00
Q85HE22	1.00
Q85HG3	1.00
D86H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN85	HA	1.00	0.003	1.00	0.65
GLN85	HB2	1.00	0.008	1.00	2.85
GLN85	HB3	1.00	0.070	0.00	0.00
GLN85	HG2	1.00	0.011	1.00	103.18
GLN85	HG3	1.00	0.011	1.00	103.18
GLN85	H	1.00	0.005	1.00	-594625.00
GLN85	HE21	1.00	0.006	1.00	-1060125.00
GLN85	HE22	1.00	1.589	0.00	0.00
ASP86	H	0.96	0.005	1.00	-238011.00

3.85.11 Detailed Probabilities of GLN85H:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP84	1.00	1.00
GLN85	0.83	1.00
ASP86	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D84HA	1.00
D84H	1.00
D84HB2	1.00
D84HB3	1.00
Q85HA	1.00
Q85HB2	1.00
Q85HB3	1.00
Q85HG2	1.00
Q85HG3	1.00
Q85H	1.00
D86H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP84	HA	1.00	0.008	1.00	1.50
ASP84	HB2	1.00	0.013	1.00	0.11
ASP84	HB3	1.00	0.012	1.00	0.13
ASP84	H	1.00	0.019	1.00	-160863.00
GLN85	HA	1.00	0.013	1.00	0.57
GLN85	HB2	1.00	0.051	0.00	0.00
GLN85	HB3	1.00	0.023	1.00	1.18
GLN85	HG2	1.00	0.011	1.00	0.69
GLN85	HG3	1.00	0.011	1.00	0.69
GLN85	H	1.00	0.005	1.00	-5727664.00
ASP86	H	1.00	0.074	0.00	0.00

3.85.12 Detailed Probabilities of GLN85HE21:

Overall probability: 0.933

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN85	0.93	1.00

Expected NOESY Contacts

Proton	Expected probability
Q85HB2	1.00
Q85HB3	1.00
Q85HG2	1.00
Q85HG3	1.00
Q85HE22	1.00
Q85HE21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN85	HB2	1.00	0.008	1.00	0.92
GLN85	HB3	1.00	0.034	0.60	0.00
GLN85	HG2	1.00	0.009	1.00	0.76
GLN85	HG3	1.00	0.009	1.00	0.76
GLN85	HE21	1.00	0.000	1.00	-33873372.00
GLN85	HE22	1.00	0.002	1.00	-15575352.00

3.85.13 Detailed Probabilities of GLN85HE22:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN85	0.83	1.00

Expected NOESY Contacts

Proton	Expected probability
Q85HB2	1.00
Q85HB3	1.00
Q85HG2	1.00
Q85HG3	1.00
Q85HE21	1.00
Q85HE22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN85	HB2	1.00	0.022	1.00	0.06
GLN85	HB3	1.00	0.019	1.00	0.09
GLN85	HG2	1.00	0.001	1.00	0.45
GLN85	HG3	1.00	0.001	1.00	0.45
GLN85	HE21	1.00	0.001	1.00	-14559339.00
GLN85	HE22	1.00	0.150	0.00	0.00

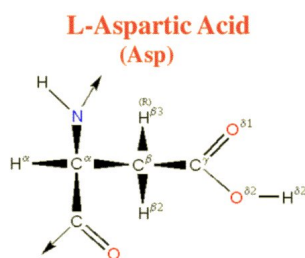
3.86 ASP(86)

Figure 85: Image from the BMRB

Residue probability: 0.574

Residue probability confidence: 0.893

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	175.747	176.463	2.348	0.000	0.000
CA 3.86.1	53.512	54.786	4.266	0.250	0.875
CB 3.86.2	40.957	40.949	3.070	0.600	0.833
N 3.86.3	120.508	120.550	5.690	0.818	1.000
HD2	NA	—	—	0.000	0.000
HA 3.86.4	4.685	4.587	0.329	0.778	0.875
HB2 3.86.5	2.927	2.708	0.282	0.600	0.833
HB3 3.86.6	2.566	2.654	0.285	0.600	0.833
H 3.86.7	8.691	8.304	1.027	0.369	1.000

3.86.1 Detailed Probabilities of ASP86CA:

Overall probability: 0.250

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN85	0.50	1.00
ASP86	0.25	0.80
GLU87	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q85HA	1.00
D86HD2	1.00
D86HB2	1.00
D86HB3	1.00
D86H	1.00
D86HA	1.00
E87H	1.00
E87HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN85	HA	1.00	0.057	0.00	0.00
GLN85	HB2	0.61	0.023	1.00	0.50
ASP86	HA	1.00	0.007	1.00	10.60
ASP86	HB2	1.00	0.173	0.00	0.00
ASP86	HB3	1.00	0.370	0.00	0.00
ASP86	H	1.00	0.186	0.00	0.00
GLU87	HA	1.00	0.052	0.00	0.00
GLU87	H	1.00	0.235	0.00	0.00

3.86.2 Detailed Probabilities of ASP86CB:

Overall probability: 0.600

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP86	0.75	0.80
GLU87	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D86HD2	1.00
D86HA	1.00
D86HB2	1.00
D86H	1.00
D86HB3	1.00
E87H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP86	HA	1.00	0.007	1.00	0.57
ASP86	HB2	1.00	0.004	1.00	3.21
ASP86	HB3	1.00	0.357	0.00	0.00
ASP86	H	1.00	0.004	1.00	0.53
GLU87	H	1.00	0.045	0.00	0.00

3.86.3 Detailed Probabilities of ASP86N:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN85	0.83	1.00
ASP86	1.00	1.00
GLU87	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q85HB3	1.00
Q85HB2	1.00
Q85H	1.00
Q85HG2	0.98
Q85HA	1.00
Q85HG3	0.96
D86HA	1.00
D86HB2	1.00
D86HB3	1.00
D86H	1.00
E87H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN85	HA	1.00	0.012	1.00	-712495.00
GLN85	HB2	1.00	0.008	1.00	-296128.00
GLN85	HB3	1.00	0.004	1.00	-460067.00
GLN85	HG2	0.98	0.003	1.00	-238011.00
GLN85	HG3	0.96	0.005	1.00	-238011.00
GLN85	H	1.00	0.074	0.00	0.00
ASP86	HA	1.00	0.009	1.00	-652254.00
ASP86	HB2	1.00	0.002	1.00	-894345.00
ASP86	HB3	1.00	0.003	1.00	-1028586.00
ASP86	H	1.00	0.000	1.00	-6795614.00
GLU87	H	1.00	0.049	0.00	0.00

3.86.4 Detailed Probabilities of ASP86HA:

Overall probability: 0.778

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN85	0.67	1.00
ASP86	0.75	0.80
GLU87	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q85HA	1.00
D86HD2	1.00
D86HB2	1.00
D86HB3	1.00
D86H	1.00
D86HA	1.00
E87H	1.00
E87HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN85	HA	1.00	0.074	0.00	0.00
GLN85	HB3	0.79	0.005	1.00	0.45
GLN85	H	0.86	0.001	1.00	-73717.00
ASP86	HA	1.00	0.007	1.00	10.60
ASP86	HB2	1.00	1.540	0.00	0.00
ASP86	HB3	1.00	0.007	1.00	0.57
ASP86	H	1.00	0.009	1.00	-652254.00
GLU87	HA	1.00	0.029	1.00	0.08
GLU87	H	1.00	0.005	1.00	-2166166.00

3.86.5 Detailed Probabilities of ASP86HB2:

Overall probability: 0.600

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP86	0.50	0.80
GLU87	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D86HD2	1.00
D86HA	1.00
D86HB3	1.00
D86H	1.00
D86HB2	1.00
E87H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP86	HA	1.00	0.173	0.00	0.00
ASP86	HB2	1.00	0.218	0.00	0.00
ASP86	HB3	1.00	0.004	1.00	3.21
ASP86	H	1.00	0.002	1.00	-894345.00
GLU87	H	1.00	0.009	1.00	-235689.00

3.86.6 Detailed Probabilities of ASP86HB3:

Overall probability: 0.600

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP86	0.50	0.80
GLU87	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D86HD2	1.00
D86HA	1.00
D86HB2	1.00
D86H	1.00
D86HB3	1.00
E87H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP86	HA	1.00	0.370	0.00	0.00
ASP86	HB2	1.00	0.000	1.00	3.11
ASP86	HB3	1.00	0.357	0.00	0.00
ASP86	H	1.00	0.003	1.00	-1028586.00
GLU87	H	1.00	0.003	1.00	-254622.00

3.86.7 Detailed Probabilities of ASP86H:

Overall probability: 0.369

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN85	0.18	1.00
ASP86	0.75	1.00
GLU87	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q85HB3	1.00
Q85HB2	1.00
Q85H	1.00
Q85HG2	0.98
Q85HA	1.00
Q85HG3	0.96
D86HA	1.00
D86HB2	1.00
D86HB3	1.00
D86H	1.00
E87H	1.00

NOESY contacts detailed probability

3.86 ASP(86)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN85	HA	1.00	0.061	0.00	0.00
GLN85	HB2	1.00	0.023	1.00	0.79
GLN85	HB3	1.00	0.595	0.00	0.00
GLN85	HG2	0.98	0.063	0.02	0.00
GLN85	HG3	0.96	0.063	0.04	0.00
GLN85	H	1.00	0.069	0.00	0.00
ASP86	HA	1.00	0.186	0.00	0.00
ASP86	HB2	1.00	0.008	1.00	0.52
ASP86	HB3	1.00	0.004	1.00	0.53
ASP86	H	1.00	0.000	1.00	-6795614.00
GLU87	H	1.00	0.043	0.00	0.00

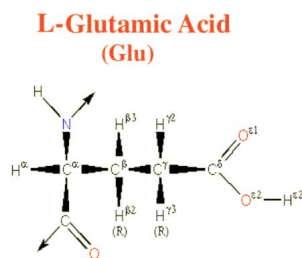


Figure 86: Image from the BMRB

Residue probability: 0.636
Residue probability confidence: 0.921

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	177.771	176.942	2.547	0.000	0.000
CA 3.87.1	58.522	57.442	3.837	0.375	1.000
CB 3.87.2	29.575	30.185	4.018	0.857	0.857
CG 3.87.3	36.010	36.085	1.533	0.833	0.857
N 3.87.4	123.604	120.574	4.837	0.800	1.000
HA 3.87.5	4.035	4.245	0.429	0.500	1.000
HB2 3.87.6	2.094	2.021	0.233	0.571	0.857
HB3 3.87.7	2.040	1.994	0.244	0.571	0.857
HG 3.87.8	2.295	2.258	0.226	0.667	0.857
H 3.87.9	8.642	8.332	0.601	0.545	1.000
HE2	NA	—	—	0.000	0.000

3.87.1 Detailed Probabilities of GLU87CA:

Overall probability: 0.375
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP86	1.00	1.00
GLU87	0.20	1.00
ASN88	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
D86HA	1.00
E87HB2	1.00
E87HB3	1.00
E87HG2	1.00
E87H	1.00
E87HA	1.00
N88HA	1.00
N88H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP86	HA	1.00	0.029	1.00	0.08
GLU87	HA	1.00	0.679	0.00	0.00
GLU87	HB2	1.00	0.834	0.00	0.00
GLU87	HB3	1.00	0.780	0.00	0.00
GLU87	HG2	1.00	1.035	0.00	0.00
GLU87	H	1.00	0.002	1.00	0.58
ASN88	HA	1.00	0.153	0.00	0.00
ASN88	H	1.00	0.013	1.00	0.37

3.87.2 Detailed Probabilities of GLU87CB:

Overall probability: 0.857

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU87	0.80	0.83
ASN88	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E87HA	1.00
E87HB3	1.00
E87HG2	1.00
E87H	1.00
E87HE2	1.00
E87HB2	1.00
N88H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU87	HA	1.00	0.001	1.00	2.70
GLU87	HB2	1.00	0.001	1.00	35.26
GLU87	HB3	1.00	0.053	0.00	0.00
GLU87	HG2	1.00	0.015	1.00	3.87
GLU87	H	1.00	0.006	1.00	0.65
ASN88	H	1.00	0.006	1.00	0.25
ASN88	HA	0.65	0.016	1.00	0.56

3.87.3 Detailed Probabilities of GLU87CG:

Overall probability: 0.833

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU87	0.80	0.83
ASN88	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E87HA	1.00
E87HB2	1.00
E87HB3	1.00
E87HG3	1.00
E87H	1.00
E87HE2	1.00
N88H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU87	HA	1.00	0.002	1.00	2.08
GLU87	HB2	1.00	0.014	1.00	8.87
GLU87	HB3	1.00	0.040	0.00	0.00
GLU87	HG2	1.00	0.001	1.00	100.68
GLU87	H	1.00	0.004	1.00	0.53
ASN88	H	0.97	0.001	1.00	0.27

3.87.4 Detailed Probabilities of GLU87N:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP86	0.75	1.00
GLU87	0.80	1.00
ASN88	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D86H	1.00
D86HA	1.00
D86HB3	1.00
D86HB2	1.00
E87HA	1.00
E87HB2	1.00
E87HB3	1.00
E87HG2	1.00
E87H	1.00
N88H	1.00

NOESY contacts detailed probability

3.87 GLU(87)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP86	HA	1.00	0.005	1.00	-2166166.00
ASP86	HB2	1.00	0.009	1.00	-235689.00
ASP86	HB3	1.00	0.003	1.00	-254622.00
ASP86	H	1.00	0.043	0.00	0.00
GLU87	HA	1.00	0.003	1.00	-853871.00
GLU87	HB2	1.00	0.058	0.00	0.00
GLU87	HB3	1.00	0.004	1.00	-1149358.00
GLU87	HG2	1.00	0.003	1.00	-743519.00
GLU87	H	1.00	0.006	1.00	-8039396.00
ASN88	H	1.00	0.010	1.00	-429726.00

3.87.5 Detailed Probabilities of GLU87HA:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP86	0.00	1.00
GLU87	0.80	1.00
ASN88	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D86HA	1.00
E87HB2	1.00
E87HB3	1.00
E87HG2	1.00
E87H	1.00
E87HA	1.00
N88HA	1.00
N88H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP86	HA	1.00	0.052	0.00	0.00
GLU87	HA	1.00	0.679	0.00	0.00
GLU87	HB2	1.00	0.001	1.00	2.70
GLU87	HB3	1.00	0.001	1.00	2.70
GLU87	HG2	1.00	0.002	1.00	2.08
GLU87	H	1.00	0.003	1.00	-853871.00
ASN88	HA	1.00	0.071	0.00	0.00
ASN88	H	1.00	0.120	0.00	0.00

3.87.6 Detailed Probabilities of GLU87HB2:

Overall probability: 0.571

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU87	0.40	0.83
ASN88	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E87HA	1.00
E87HB3	1.00
E87HG2	1.00
E87H	1.00
E87HE2	1.00
E87HB2	1.00
N88H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU87	HA	1.00	0.834	0.00	0.00
GLU87	HB2	1.00	0.001	1.00	35.26
GLU87	HB3	1.00	0.053	0.00	0.00
GLU87	HG2	1.00	0.014	1.00	8.87
GLU87	H	1.00	0.058	0.00	0.00
ASN88	H	1.00	0.003	1.00	-571030.00
ASN88	HA	0.65	0.001	1.00	0.98

3.87.7 Detailed Probabilities of GLU87HB3:

Overall probability: 0.571

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU87	0.40	0.83
ASN88	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E87HA	1.00
E87HB2	1.00
E87HG2	1.00
E87H	1.00
E87HE2	1.00
E87HB3	1.00
N88H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU87	HA	1.00	0.780	0.00	0.00
GLU87	HB2	1.00	0.053	0.00	0.00
GLU87	HB3	1.00	0.001	1.00	52.03
GLU87	HG2	1.00	0.040	0.00	0.00
GLU87	H	1.00	0.004	1.00	-1149358.00
ASN88	H	1.00	0.007	1.00	-552799.00
ASN88	HB2	0.50	0.007	1.00	0.13

3.87.8 Detailed Probabilities of GLU87HG2:

Overall probability: 0.667

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU87	0.60	0.83
ASN88	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E87HA	1.00
E87HB2	1.00
E87HB3	1.00
E87HG3	1.00
E87H	1.00
E87HE2	1.00
N88H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU87	HA	1.00	1.035	0.00	0.00
GLU87	HB2	1.00	0.015	1.00	3.87
GLU87	HB3	1.00	0.040	0.00	0.00
GLU87	HG2	1.00	0.001	1.00	100.68
GLU87	H	1.00	0.003	1.00	-743519.00
ASN88	H	0.97	0.010	1.00	-359269.00

3.87.9 Detailed Probabilities of GLU87H:

Overall probability: 0.545

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP86	0.00	1.00
GLU87	1.00	1.00
ASN88	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
D86H	1.00
D86HA	1.00
D86HB3	1.00
D86HB2	1.00
E87HA	1.00
E87HB2	1.00
E87HB3	1.00
E87HG2	1.00
E87H	1.00
N88H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP86	HA	1.00	0.235	0.00	0.00
ASP86	HB2	1.00	0.041	0.00	0.00
ASP86	HB3	1.00	0.045	0.00	0.00
ASP86	H	1.00	0.049	0.00	0.00
GLU87	HA	1.00	0.002	1.00	0.58
GLU87	HB2	1.00	0.006	1.00	0.65
GLU87	HB3	1.00	0.002	1.00	1.18
GLU87	HG2	1.00	0.004	1.00	0.53
GLU87	H	1.00	0.006	1.00	-8039396.00
ASN88	H	1.00	0.416	0.00	0.00
ASN88	HB2	0.65	0.012	1.00	0.05

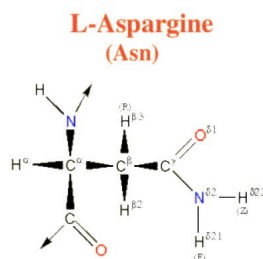
3.88 ASN(88)

Figure 87: Image from the BMRB

Residue probability: 0.660
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	177.089	175.315	1.862	0.000	0.000
CA 3.88.1	55.642	53.674	5.429	0.480	1.000
CB 3.88.2	38.166	38.785	5.449	0.750	1.000
N 3.88.3	118.838	118.907	6.480	0.692	1.000
ND2 3.88.4	114.317	112.932	14.355	0.833	1.000
HA 3.88.5	4.561	4.658	0.371	0.799	1.000
HB2 3.88.6	2.850	2.800	0.341	0.143	1.000
HB3 3.88.7	2.905	2.739	0.364	0.686	1.000
H 3.88.8	8.527	8.328	0.633	0.750	1.000
HD21 3.88.9	7.890	7.343	1.188	0.667	1.000
HD22 3.88.10	7.028	7.145	1.184	0.800	1.000

3.88.1 Detailed Probabilities of ASN88CA:

Overall probability: 0.480
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU87	0.50	1.00
ASN88	0.47	1.00
GLU89	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E87HA	1.00
N88HB2	1.00
N88HB3	1.00
N88H	1.00
N88HD21	1.00
N88HD22	1.00
N88HA	1.00
E89H	1.00
E89HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU87	HA	1.00	0.071	0.00	0.00
GLU87	HB2	0.65	0.001	1.00	0.98
ASN88	HA	1.00	0.022	1.00	90.61
ASN88	HB2	1.00	0.011	1.00	1.70
ASN88	HB3	1.00	0.032	0.80	0.00
ASN88	H	1.00	0.076	0.00	0.00
ASN88	HD21	1.00	0.088	0.00	0.00
ASN88	HD22	1.00	0.073	0.00	0.00
GLU89	HA	1.00	0.173	0.00	0.00
GLU89	H	1.00	0.005	1.00	0.40

3.88.2 Detailed Probabilities of ASN88CB:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN88	0.67	1.00
GLU89	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N88HA	1.00
N88HB2	1.00
N88H	1.00
N88HD21	1.00
N88HD22	1.00
N88HB3	1.00
E89H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN88	HA	1.00	0.009	1.00	1.05
ASN88	HB2	1.00	0.290	0.00	0.00
ASN88	HB3	1.00	0.345	0.00	0.00
ASN88	H	1.00	0.005	1.00	0.50
ASN88	HD21	1.00	0.010	1.00	0.32
ASN88	HD22	1.00	0.001	1.00	0.10
GLU89	H	1.00	0.019	1.00	0.26
GLU89	HA	0.83	0.008	1.00	0.07

3.88.3 Detailed Probabilities of ASN88N:

Overall probability: 0.692

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU87	0.60	1.00
ASN88	0.60	1.00
GLU89	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E87HG2	0.98
E87HB3	1.00
E87HB2	1.00
E87HA	1.00
E87H	1.00
N88HA	1.00
N88HB2	1.00
N88HB3	1.00
N88HD21	0.98
N88H	1.00
E89H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU87	HA	1.00	0.120	0.00	0.00
GLU87	HB2	1.00	0.003	1.00	-571030.00
GLU87	HB3	1.00	0.007	1.00	-552799.00
GLU87	HG2	0.98	0.010	1.00	-359269.00
GLU87	H	1.00	0.416	0.00	0.00
ASN88	HA	1.00	0.015	1.00	-737454.00
ASN88	HB2	1.00	0.056	0.00	0.00
ASN88	HB3	1.00	0.001	1.00	-1179261.00
ASN88	H	1.00	0.301	0.00	0.00
ASN88	HD21	0.98	0.012	1.00	-101385.00
GLU89	H	1.00	0.005	1.00	-763241.00
GLU89	HA	0.89	0.008	1.00	-182461.00
GLU89	HB2	0.58	0.007	1.00	-552799.00

3.88.4 Detailed Probabilities of ASN88ND2:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN88	0.83	1.00

Expected NOESY Contacts

Proton	Expected probability
N88HA	1.00
N88HB2	1.00
N88HB3	1.00
N88H	0.98
N88HD22	1.00
N88HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN88	HA	1.00	0.010	1.00	-149589.00
ASN88	HB2	1.00	0.056	0.00	0.00
ASN88	HB3	1.00	0.001	1.00	-796098.00
ASN88	H	0.98	0.002	1.00	-147324.00
ASN88	HD21	1.00	0.004	1.00	-17795558.00
ASN88	HD22	1.00	0.005	1.00	-11854401.00

3.88.5 Detailed Probabilities of ASN88HA:

Overall probability: 0.799

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU87	0.59	1.00
ASN88	1.00	1.00
GLU89	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E87HA	1.00
N88HB2	1.00
N88HB3	1.00
N88H	1.00
N88HD21	1.00
N88HD22	1.00
N88HA	1.00
E89H	1.00
E89HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU87	HA	1.00	0.153	0.00	0.00
GLU87	HB2	0.65	0.016	1.00	0.56
GLU87	HB3	0.78	0.033	0.78	0.00
ASN88	HA	1.00	0.022	1.00	90.61
ASN88	HB2	1.00	0.007	1.00	1.14
ASN88	HB3	1.00	0.009	1.00	1.05
ASN88	H	1.00	0.015	1.00	-737454.00
ASN88	HD21	1.00	0.010	1.00	-149589.00
ASN88	HD22	1.00	0.011	1.00	-122792.00
GLU89	HA	1.00	0.416	0.00	0.00
GLU89	H	1.00	0.014	1.00	-421029.00

3.88.6 Detailed Probabilities of ASN88HB2:

Overall probability: 0.143

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN88	0.17	1.00
GLU89	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N88HA	1.00
N88HB3	1.00
N88H	1.00
N88HD21	1.00
N88HD22	1.00
N88HB2	1.00
E89H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN88	HA	1.00	0.011	1.00	1.70
ASN88	HB2	1.00	0.180	0.00	0.00
ASN88	HB3	1.00	0.290	0.00	0.00
ASN88	H	1.00	0.056	0.00	0.00
ASN88	HD21	1.00	0.056	0.00	0.00
ASN88	HD22	1.00	0.059	0.00	0.00
GLU89	H	1.00	0.061	0.00	0.00

3.88.7 Detailed Probabilities of ASN88HB3:

Overall probability: 0.686

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN88	0.63	1.00
GLU89	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N88HA	1.00
N88HB2	1.00
N88H	1.00
N88HD21	1.00
N88HD22	1.00
N88HB3	1.00
E89H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN88	HA	1.00	0.032	0.80	0.00
ASN88	HB2	1.00	0.235	0.00	0.00
ASN88	HB3	1.00	0.345	0.00	0.00
ASN88	H	1.00	0.001	1.00	-1179261.00
ASN88	HD21	1.00	0.001	1.00	-796098.00
ASN88	HD22	1.00	0.004	1.00	-497036.00
GLU89	H	1.00	0.006	1.00	-511040.00

3.88.8 Detailed Probabilities of ASN88H:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU87	0.80	1.00
ASN88	0.67	1.00
GLU89	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E87HG2	0.98
E87HB3	1.00
E87HB2	1.00
E87HA	1.00
E87H	1.00
N88HA	1.00
N88HB2	1.00
N88HB3	1.00
N88HD21	0.98
N88H	1.00
E89H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU87	HA	1.00	0.013	1.00	0.37
GLU87	HB2	1.00	0.006	1.00	0.25
GLU87	HB3	1.00	0.113	0.00	0.00
GLU87	HG2	0.98	0.001	1.00	0.27
GLU87	H	1.00	0.010	1.00	-429726.00
ASN88	HA	1.00	0.076	0.00	0.00
ASN88	HB2	1.00	0.006	1.00	0.61
ASN88	HB3	1.00	0.005	1.00	0.50
ASN88	H	1.00	0.301	0.00	0.00
ASN88	HD21	0.98	0.002	1.00	-147324.00
ASN88	HD22	0.63	0.022	1.00	-78476.00
GLU89	H	1.00	0.010	1.00	-548642.00

3.88.9 Detailed Probabilities of ASN88HD21:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN88	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
N88HA	1.00
N88HB2	1.00
N88HB3	1.00
N88H	0.98
N88HD22	1.00
N88HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN88	HA	1.00	0.088	0.00	0.00
ASN88	HB2	1.00	0.349	0.00	0.00
ASN88	HB3	1.00	0.010	1.00	0.32
ASN88	H	0.98	0.012	1.00	-101385.00
ASN88	HD21	1.00	0.004	1.00	-17795558.00
ASN88	HD22	1.00	0.005	1.00	-12958762.00

3.88.10 Detailed Probabilities of ASN88HD22:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN88	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
N88HA	1.00
N88HB2	1.00
N88HB3	1.00
N88HD21	1.00
N88HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN88	HA	1.00	0.073	0.00	0.00
ASN88	HB2	1.00	0.004	1.00	0.17
ASN88	HB3	1.00	0.001	1.00	0.10
ASN88	HD21	1.00	0.005	1.00	-11854401.00
ASN88	HD22	1.00	0.005	1.00	-22611540.00

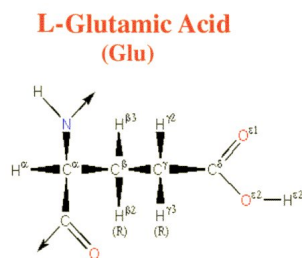
3.89 GLU(89)

Figure 88: Image from the BMRB

Residue probability: 0.701

Residue probability confidence: 0.921

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.357	176.942	2.547	0.000	0.000
CA 3.89.1	58.251	57.442	3.837	0.500	1.000
CB 3.89.2	29.244	30.185	4.018	0.667	0.857
CG 3.89.3	36.010	36.085	1.533	0.621	0.857
N 3.89.4	120.947	120.574	4.837	0.818	1.000
HA 3.89.5	4.147	4.245	0.429	0.727	1.000
HB 3.89.6	2.040	2.021	0.233	0.667	0.857
HG2 3.89.7	2.263	2.258	0.226	0.733	0.857
HG3 3.89.8	2.311	2.233	0.232	0.667	0.857
H 3.89.9	8.221	8.332	0.601	0.909	1.000
HE2	NA	—	—	0.000	0.000

3.89.1 Detailed Probabilities of GLU89CA:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN88	0.00	1.00
GLU89	0.60	1.00
LEU90	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
N88HA	1.00
E89HB2	1.00
E89HG2	1.00
E89HG3	1.00
E89H	1.00
E89HA	1.00
L90H	1.00
L90HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN88	HA	1.00	0.416	0.00	0.00
GLU89	HA	1.00	0.002	1.00	24.81
GLU89	HB2	1.00	0.007	1.00	2.44
GLU89	HG2	1.00	0.014	1.00	2.15
GLU89	HG3	1.00	0.062	0.00	0.00
GLU89	H	1.00	0.105	0.00	0.00
LEU90	HA	1.00	0.060	0.00	0.00
LEU90	H	1.00	0.015	1.00	1.25

3.89.2 Detailed Probabilities of GLU89CB:

Overall probability: 0.667

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU89	0.80	0.83
LEU90	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E89HA	1.00
E89HB3	1.00
E89HG2	1.00
E89HG3	1.00
E89H	1.00
E89HE2	1.00
L90H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU89	HA	1.00	0.003	1.00	2.48
GLU89	HB2	1.00	0.001	1.00	52.03
GLU89	HG2	1.00	0.072	0.00	0.00
GLU89	HG3	1.00	0.024	1.00	4.32
GLU89	H	1.00	0.005	1.00	1.39
LEU90	H	1.00	0.049	0.00	0.00

3.89.3 Detailed Probabilities of GLU89CG:

Overall probability: 0.621

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU89	0.74	0.83
LEU90	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
E89HA	1.00
E89HB2	1.00
E89HG2	1.00
E89H	1.00
E89HE2	1.00
E89HG3	1.00
L90H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU89	HA	1.00	0.006	1.00	0.69
GLU89	HB2	1.00	0.040	0.00	0.00
GLU89	HG2	1.00	0.033	0.70	0.00
GLU89	HG3	1.00	0.015	1.00	100.68
GLU89	H	1.00	0.008	1.00	1.06
LEU90	H	0.97	0.050	0.03	0.00

3.89.4 Detailed Probabilities of GLU89N:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN88	0.75	1.00
GLU89	0.80	1.00
LEU90	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N88HB2	1.00
N88HA	1.00
N88HB3	1.00
N88H	1.00
E89HA	1.00
E89HB2	1.00
E89HG2	1.00
E89HG3	1.00
E89H	1.00
L90H	1.00

NOESY contacts detailed probability

3.89 GLU(89)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN88	HA	1.00	0.014	1.00	-421029.00
ASN88	HB2	1.00	0.061	0.00	0.00
ASN88	HB3	1.00	0.006	1.00	-511040.00
ASN88	H	1.00	0.010	1.00	-548642.00
GLU89	HA	1.00	0.000	1.00	-750944.00
GLU89	HB2	1.00	0.009	1.00	-1497819.00
GLU89	HG2	1.00	0.008	1.00	-387045.00
GLU89	HG3	1.00	0.040	0.00	0.00
GLU89	H	1.00	0.005	1.00	-5432360.00
LEU90	H	1.00	0.010	1.00	-602840.00
LEU90	HB2	0.69	0.006	1.00	-86513.00

3.89.5 Detailed Probabilities of GLU89HA:

Overall probability: 0.727

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN88	0.75	1.00
GLU89	1.00	1.00
LEU90	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N88HA	1.00
E89HB2	1.00
E89HG2	1.00
E89HG3	1.00
E89H	1.00
E89HA	1.00
L90H	1.00
L90HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN88	HA	1.00	0.173	0.00	0.00
ASN88	HB2	0.62	0.004	1.00	0.08
ASN88	HB3	0.83	0.008	1.00	0.07
ASN88	H	0.89	0.008	1.00	-182461.00
GLU89	HA	1.00	0.002	1.00	24.81
GLU89	HB2	1.00	0.003	1.00	2.48
GLU89	HG2	1.00	0.006	1.00	0.74
GLU89	HG3	1.00	0.006	1.00	0.69
GLU89	H	1.00	0.000	1.00	-750944.00
LEU90	HA	1.00	0.057	0.00	0.00
LEU90	H	1.00	0.046	0.00	0.00

3.89.6 Detailed Probabilities of GLU89HB2:

Overall probability: 0.667

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU89	0.60	0.83
LEU90	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E89HA	1.00
E89HB3	1.00
E89HG2	1.00
E89HG3	1.00
E89H	1.00
E89HE2	1.00
L90H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU89	HA	1.00	0.007	1.00	2.44
GLU89	HB2	1.00	0.001	1.00	52.03
GLU89	HG2	1.00	0.040	0.00	0.00
GLU89	HG3	1.00	0.040	0.00	0.00
GLU89	H	1.00	0.009	1.00	-1497819.00
LEU90	H	1.00	0.007	1.00	-904565.00

3.89.7 Detailed Probabilities of GLU89HG2:

Overall probability: 0.733

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU89	0.68	0.83
LEU90	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E89HA	1.00
E89HB2	1.00
E89HG3	1.00
E89H	1.00
E89HE2	1.00
E89HG2	1.00
L90H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU89	HA	1.00	0.014	1.00	2.15
GLU89	HB2	1.00	0.072	0.00	0.00
GLU89	HG2	1.00	0.033	0.70	0.00
GLU89	HG3	1.00	0.033	0.70	0.00
GLU89	H	1.00	0.008	1.00	-387045.00
LEU90	H	0.98	0.026	1.00	-193405.00

3.89.8 Detailed Probabilities of GLU89HG3:

Overall probability: 0.667

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU89	0.60	0.83
LEU90	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E89HA	1.00
E89HB2	1.00
E89HG2	1.00
E89H	1.00
E89HE2	1.00
E89HG3	1.00
L90H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU89	HA	1.00	0.062	0.00	0.00
GLU89	HB2	1.00	0.024	1.00	4.32
GLU89	HG2	1.00	0.015	1.00	100.68
GLU89	HG3	1.00	0.015	1.00	100.68
GLU89	H	1.00	0.040	0.00	0.00
LEU90	H	0.97	0.022	1.00	-193405.00

3.89.9 Detailed Probabilities of GLU89H:

Overall probability: 0.909

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASN88	1.00	1.00
GLU89	0.80	1.00
LEU90	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
N88HB2	1.00
N88HA	1.00
N88HB3	1.00
N88H	1.00
E89HA	1.00
E89HB2	1.00
E89HG2	1.00
E89HG3	1.00
E89H	1.00
L90H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASN88	HA	1.00	0.005	1.00	0.40
ASN88	HB2	1.00	0.018	1.00	0.29
ASN88	HB3	1.00	0.019	1.00	0.26
ASN88	H	1.00	0.005	1.00	-763241.00
GLU89	HA	1.00	0.105	0.00	0.00
GLU89	HB2	1.00	0.005	1.00	1.39
GLU89	HG2	1.00	0.004	1.00	0.66
GLU89	HG3	1.00	0.008	1.00	1.06
GLU89	H	1.00	0.005	1.00	-5432360.00
LEU90	H	1.00	0.005	1.00	-761175.00
LEU90	HA	0.93	0.022	1.00	0.07

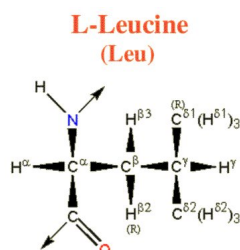
3.90 LEU(90)

Figure 89: Image from the BMRB

Residue probability: 0.788

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	177.917	177.056	1.929	0.000	0.000
CA 3.90.1	56.944	55.735	3.802	0.619	1.000
CB 3.90.2	42.456	42.389	3.750	0.889	1.000
CG 3.90.3	26.770	26.892	3.086	0.875	1.000
CD1 3.90.4	24.861	24.837	3.657	0.857	1.000
CD2 3.90.5	24.744	24.201	3.117	0.857	1.000
N 3.90.6	119.582	121.785	4.943	0.914	1.000
HA 3.90.7	4.205	4.315	0.840	0.800	1.000
HB2 3.90.8	1.776	1.601	0.373	0.625	1.000
HB3 3.90.9	1.722	1.508	0.398	0.700	1.000
HG 3.90.10	1.639	1.510	0.340	0.628	1.000
HD1 3.90.11	0.903	0.739	0.294	0.858	1.000
HD2 3.90.12	0.882	0.727	0.421	0.858	1.000
H 3.90.13	8.047	8.237	0.647	0.757	1.000

3.90.1 Detailed Probabilities of LEU90CA:

Overall probability: 0.619

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU89	0.50	1.00
LEU90	0.69	1.00
GLU91	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E89HA	1.00
L90HB2	1.00
L90HB3	1.00
L90HG	1.00
L90HD11	0.99
L90HD21	0.99
L90H	1.00
L90HA	1.00
E91HA	1.00
E91H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU89	HA	1.00	0.057	0.00	0.00
GLU89	H	0.93	0.022	1.00	0.07
LEU90	HA	1.00	0.001	1.00	9.24
LEU90	HB2	1.00	0.022	1.00	0.71
LEU90	HB3	1.00	0.032	0.80	0.00
LEU90	HG	1.00	0.022	1.00	0.47
LEU90	HD11	0.99	0.547	0.01	0.00
LEU90	HD21	0.99	0.568	0.01	0.00
LEU90	H	1.00	0.016	1.00	0.54
GLU91	HA	1.00	0.131	0.00	0.00
GLU91	H	1.00	0.006	1.00	0.22

3.90.2 Detailed Probabilities of LEU90CB:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU90	0.86	1.00
GLU91	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L90HA	1.00
L90HB3	1.00
L90HG	1.00
L90HD11	1.00
L90HD21	1.00
L90H	1.00
L90HB2	1.00
E91H	1.00

NOESY contacts detailed probability

3.90 LEU(90)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU90	HA	1.00	0.001	1.00	0.34
LEU90	HB2	1.00	0.024	1.00	1.98
LEU90	HB3	1.00	0.030	1.00	0.00
LEU90	HG	1.00	0.113	0.00	0.00
LEU90	HD11	1.00	0.012	1.00	0.97
LEU90	HD21	1.00	0.009	1.00	0.97
LEU90	H	1.00	0.011	1.00	0.44
GLU91	H	1.00	0.004	1.00	0.19
GLU91	HA	0.72	0.026	1.00	0.18

3.90.3 Detailed Probabilities of LEU90CG:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU90	0.86	1.00
GLU91	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L90HA	1.00
L90HB2	1.00
L90HB3	1.00
L90HD11	1.00
L90HD21	1.00
L90H	1.00
L90HG	1.00
E91H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU90	HA	1.00	0.007	1.00	0.23
LEU90	HB2	1.00	0.011	1.00	2.53
LEU90	HB3	1.00	0.043	0.00	0.00
LEU90	HG	1.00	0.003	1.00	19.97
LEU90	HD11	1.00	0.021	1.00	1.97
LEU90	HD21	1.00	0.000	1.00	1.97
LEU90	H	1.00	0.008	1.00	0.53
GLU91	H	0.98	0.001	1.00	0.11

3.90.4 Detailed Probabilities of LEU90CD1:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU90	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
L90HA	0.99
L90HB2	1.00
L90HB3	1.00
L90HG	1.00
L90HD12	1.00
L90HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU90	HA	0.99	0.001	1.00	1.50
LEU90	HB2	1.00	0.044	0.00	0.00
LEU90	HB3	1.00	0.010	1.00	2.96
LEU90	HG	1.00	0.003	1.00	3.36
LEU90	HD11	1.00	0.001	1.00	147.68
LEU90	HD21	1.00	0.020	1.00	147.68
LEU90	H	0.86	0.019	1.00	0.43

3.90.5 Detailed Probabilities of LEU90CD2:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU90	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
L90HA	0.99
L90HB2	1.00
L90HB3	1.00
L90HG	1.00
L90HD11	1.00
L90HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU90	HA	0.99	0.001	1.00	1.50
LEU90	HB2	1.00	0.044	0.00	0.00
LEU90	HB3	1.00	0.010	1.00	2.96
LEU90	HG	1.00	0.003	1.00	3.36
LEU90	HD11	1.00	0.001	1.00	147.68
LEU90	HD21	1.00	0.020	1.00	147.68
LEU90	H	0.85	0.019	1.00	0.43

3.90.6 Detailed Probabilities of LEU90N:

Overall probability: 0.914

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU89	0.80	1.00
LEU90	0.97	1.00
GLU91	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E89HB2	1.00
E89HG2	0.98
E89HG3	0.97
E89H	1.00
E89HA	1.00
L90HA	1.00
L90HB2	1.00
L90HB3	1.00
L90HG	1.00
L90H	1.00
E91H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU89	HA	1.00	0.046	0.00	0.00
GLU89	HB2	1.00	0.007	1.00	-904565.00
GLU89	HG2	0.98	0.026	1.00	-193405.00
GLU89	HG3	0.97	0.022	1.00	-193405.00
GLU89	H	1.00	0.005	1.00	-761175.00
LEU90	HA	1.00	0.012	1.00	-782459.00
LEU90	HB2	1.00	0.022	1.00	-1240230.00
LEU90	HB3	1.00	0.032	0.80	0.00
LEU90	HG	1.00	0.013	1.00	-733364.00
LEU90	H	1.00	0.009	1.00	-7986668.00
LEU90	HD11	0.88	0.014	1.00	-691194.00
LEU90	HD21	0.87	0.007	1.00	-691194.00
GLU91	H	1.00	0.006	1.00	-673755.00
GLU91	HA	0.90	0.027	1.00	-290946.00

3.90.7 Detailed Probabilities of LEU90HA:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU89	0.00	1.00
LEU90	1.00	1.00
GLU91	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E89HA	1.00
L90HB2	1.00
L90HB3	1.00
L90HG	1.00
L90HD11	0.99
L90HD21	0.99
L90H	1.00
L90HA	1.00
E91HA	1.00
E91H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU89	HA	1.00	0.060	0.00	0.00
LEU90	HA	1.00	0.001	1.00	9.24
LEU90	HB2	1.00	0.001	1.00	0.34
LEU90	HB3	1.00	0.002	1.00	0.33
LEU90	HG	1.00	0.007	1.00	0.23
LEU90	HD11	0.99	0.001	1.00	1.50
LEU90	HD21	0.99	0.001	1.00	1.50
LEU90	H	1.00	0.012	1.00	-782459.00
GLU91	HA	1.00	0.163	0.00	0.00
GLU91	H	1.00	0.006	1.00	-315049.00

3.90.8 Detailed Probabilities of LEU90HB2:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU90	0.57	1.00
GLU91	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L90HA	1.00
L90HB3	1.00
L90HG	1.00
L90HD11	1.00
L90HD21	1.00
L90H	1.00
L90HB2	1.00
E91H	1.00

NOESY contacts detailed probability

3.90 LEU(90)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU90	HA	1.00	0.022	1.00	0.71
LEU90	HB2	1.00	0.024	1.00	1.98
LEU90	HB3	1.00	0.268	0.00	0.00
LEU90	HG	1.00	0.011	1.00	2.53
LEU90	HD11	1.00	0.044	0.00	0.00
LEU90	HD21	1.00	0.044	0.00	0.00
LEU90	H	1.00	0.022	1.00	-1240230.00
GLU91	H	1.00	0.027	1.00	-568404.00

3.90.9 Detailed Probabilities of LEU90HB3:

Overall probability: 0.700

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU90	0.66	1.00
GLU91	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L90HA	1.00
L90HB2	1.00
L90HG	1.00
L90HD11	1.00
L90HD21	1.00
L90H	1.00
L90HB3	1.00
E91H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU90	HA	1.00	0.032	0.80	0.00
LEU90	HB2	1.00	0.030	1.00	0.00
LEU90	HB3	1.00	0.322	0.00	0.00
LEU90	HG	1.00	0.043	0.00	0.00
LEU90	HD11	1.00	0.010	1.00	2.96
LEU90	HD21	1.00	0.010	1.00	2.96
LEU90	H	1.00	0.032	0.80	0.00
GLU91	H	1.00	0.027	1.00	-568404.00

3.90.10 Detailed Probabilities of LEU90HG:

Overall probability: 0.628

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU90	0.71	1.00
GLU91	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
L90HA	1.00
L90HB2	1.00
L90HB3	1.00
L90HD11	1.00
L90HD21	1.00
L90H	1.00
L90HG	1.00
E91H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU90	HA	1.00	0.022	1.00	0.47
LEU90	HB2	1.00	0.113	0.00	0.00
LEU90	HB3	1.00	0.405	0.00	0.00
LEU90	HG	1.00	0.003	1.00	19.97
LEU90	HD11	1.00	0.003	1.00	3.36
LEU90	HD21	1.00	0.003	1.00	3.36
LEU90	H	1.00	0.013	1.00	-733364.00
GLU91	H	0.98	0.110	0.02	0.00

3.90.11 Detailed Probabilities of LEU90HD11:

Overall probability: 0.858

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU90	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
L90HA	0.99
L90HB2	1.00
L90HB3	1.00
L90HG	1.00
L90HD12	1.00
L90HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU90	HA	0.99	0.547	0.01	0.00
LEU90	HB2	1.00	0.012	1.00	0.97
LEU90	HB3	1.00	0.013	1.00	0.90
LEU90	HG	1.00	0.021	1.00	1.97
LEU90	HD11	1.00	0.001	1.00	147.68
LEU90	HD21	1.00	0.001	1.00	147.68
LEU90	H	0.86	0.014	1.00	-691194.00

3.90.12 Detailed Probabilities of LEU90HD21:

Overall probability: 0.858

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU90	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
L90HA	0.99
L90HB2	1.00
L90HB3	1.00
L90HG	1.00
L90HD11	1.00
L90HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU90	HA	0.99	0.568	0.01	0.00
LEU90	HB2	1.00	0.009	1.00	0.97
LEU90	HB3	1.00	0.008	1.00	0.90
LEU90	HG	1.00	0.000	1.00	1.97
LEU90	HD11	1.00	0.020	1.00	147.68
LEU90	HD21	1.00	0.020	1.00	147.68
LEU90	H	0.85	0.007	1.00	-691194.00

3.90.13 Detailed Probabilities of LEU90H:

Overall probability: 0.757

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU89	0.41	1.00
LEU90	1.00	1.00
GLU91	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
E89HB2	1.00
E89HG2	0.98
E89HG3	0.97
E89H	1.00
E89HA	1.00
L90HA	1.00
L90HB2	1.00
L90HB3	1.00
L90HG	1.00
L90H	1.00
E91H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU89	HA	1.00	0.015	1.00	1.25
GLU89	HB2	1.00	0.049	0.00	0.00
GLU89	HG2	0.98	0.049	0.02	0.00
GLU89	HG3	0.97	0.050	0.03	0.00
GLU89	H	1.00	0.010	1.00	-602840.00
LEU90	HA	1.00	0.016	1.00	0.54
LEU90	HB2	1.00	0.011	1.00	0.44
LEU90	HB3	1.00	0.012	1.00	0.42
LEU90	HG	1.00	0.008	1.00	0.53
LEU90	H	1.00	0.009	1.00	-7986668.00
LEU90	HD11	0.88	0.019	1.00	0.43
LEU90	HD21	0.87	0.019	1.00	0.43
GLU91	H	1.00	0.032	0.80	0.00

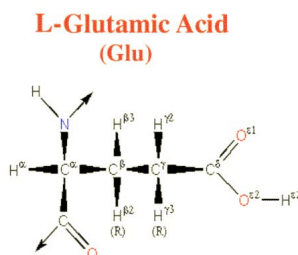


Figure 90: Image from the BMRB

Residue probability: 0.675
Residue probability confidence: 0.925

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.284	176.942	2.547	0.000	0.000
CA 3.91.1	59.129	57.442	3.837	0.767	1.000
CB 3.91.2	28.970	30.185	4.018	0.887	0.875
CG 3.91.3	35.054	36.085	1.533	0.147	0.875
N 3.91.4	119.029	120.574	4.837	0.887	1.000
HA 3.91.5	4.073	4.245	0.429	0.592	1.000
HB2 3.91.6	2.125	2.021	0.233	0.486	0.875
HB3 3.91.7	2.069	1.994	0.244	0.700	0.875
HG2 3.91.8	2.417	2.258	0.226	0.574	0.875
HG3 3.91.9	2.287	2.233	0.232	0.714	0.875
H 3.91.10	7.940	8.332	0.601	1.000	1.000
HE2	NA	—	—	0.000	0.000

3.91.1 Detailed Probabilities of GLU91CA:

Overall probability: 0.767
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU90	0.00	1.00
GLU91	0.82	1.00
GLU92	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L90HA	1.00
E91HB2	1.00
E91HB3	1.00
E91HG2	1.00
E91HG3	1.00
E91H	1.00
E91HA	1.00
E92H	1.00
E92HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU90	HA	1.00	0.163	0.00	0.00
GLU91	HA	1.00	0.031	0.90	0.00
GLU91	HB2	1.00	0.040	0.00	0.00
GLU91	HB3	1.00	0.009	1.00	5.05
GLU91	HG2	1.00	0.007	1.00	1.54
GLU91	HG3	1.00	0.005	1.00	2.14
GLU91	H	1.00	0.002	1.00	0.75
GLU92	HA	1.00	0.010	1.00	41.95
GLU92	H	1.00	0.004	1.00	1.04

3.91.2 Detailed Probabilities of GLU91CB:

Overall probability: 0.887

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU91	0.85	0.86
GLU92	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E91HA	1.00
E91HB2	1.00
E91HG2	1.00
E91HG3	1.00
E91H	1.00
E91HE2	1.00
E91HB3	1.00
E92H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU91	HA	1.00	0.037	0.30	0.00
GLU91	HB2	1.00	0.032	0.80	0.00
GLU91	HB3	1.00	0.024	1.00	35.26
GLU91	HG2	1.00	0.013	1.00	2.04
GLU91	HG3	1.00	0.007	1.00	3.87
GLU91	H	1.00	0.004	1.00	1.51
GLU92	H	1.00	0.015	1.00	1.50
GLU92	HA	0.81	0.004	1.00	2.70

3.91.3 Detailed Probabilities of GLU91CG:

Overall probability: 0.147

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU91	0.17	0.86
GLU92	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
E91HA	1.00
E91HB2	1.00
E91HB3	1.00
E91HG2	1.00
E91H	1.00
E91HE2	1.00
E91HG3	1.00
E92H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU91	HA	1.00	0.501	0.00	0.00
GLU91	HB2	1.00	2.449	0.00	0.00
GLU91	HB3	1.00	2.505	0.00	0.00
GLU91	HG2	1.00	2.157	0.00	0.00
GLU91	HG3	1.00	2.287	0.00	0.00
GLU91	H	1.00	0.010	1.00	0.24
GLU92	H	0.97	0.138	0.03	0.00

3.91.4 Detailed Probabilities of GLU91N:

Overall probability: 0.887

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU90	0.83	1.00
GLU91	0.93	1.00
GLU92	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L90HA	1.00
L90HB2	1.00
L90HB3	1.00
L90HG	0.98
L90H	1.00
E91HA	1.00
E91HB2	1.00
E91HB3	1.00
E91HG2	1.00
E91HG3	1.00
E91H	1.00
E92H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU90	HA	1.00	0.006	1.00	-315049.00
LEU90	HB2	1.00	0.027	1.00	-568404.00
LEU90	HB3	1.00	0.027	1.00	-568404.00
LEU90	HG	0.98	0.110	0.02	0.00
LEU90	H	1.00	0.032	0.80	0.00
LEU90	HD11	0.51	0.011	1.00	-244504.00
LEU90	HD21	0.58	0.010	1.00	-244504.00
GLU91	HA	1.00	0.007	1.00	-712579.00
GLU91	HB2	1.00	0.022	1.00	-1483442.00
GLU91	HB3	1.00	0.034	0.60	0.00
GLU91	HG2	1.00	0.000	1.00	-393850.00
GLU91	HG3	1.00	0.000	1.00	-484603.00
GLU91	H	1.00	0.004	1.00	-8035352.00
GLU92	H	1.00	0.009	1.00	-1240238.00

3.91.5 Detailed Probabilities of GLU91HA:

Overall probability: 0.592

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU90	0.75	1.00
GLU91	0.37	1.00
GLU92	0.95	1.00

Expected NOESY Contacts

Proton	Expected probability
L90HA	1.00
E91HB2	1.00
E91HB3	1.00
E91HG2	1.00
E91HG3	1.00
E91H	1.00
E91HA	1.00
E92H	1.00
E92HA	1.00

NOESY contacts detailed probability

3.91 GLU(91)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU90	HA	1.00	0.131	0.00	0.00
LEU90	HB2	0.72	0.026	1.00	0.18
LEU90	HB3	0.90	0.029	1.00	0.19
LEU90	H	0.90	0.027	1.00	-290946.00
GLU91	HA	1.00	0.031	0.90	0.00
GLU91	HB2	1.00	0.260	0.00	0.00
GLU91	HB3	1.00	0.037	0.30	0.00
GLU91	HG2	1.00	0.853	0.00	0.00
GLU91	HG3	1.00	0.501	0.00	0.00
GLU91	H	1.00	0.007	1.00	-712579.00
GLU92	HA	1.00	0.031	0.90	0.00
GLU92	H	1.00	0.022	1.00	-909549.00

3.91.6 Detailed Probabilities of GLU91HB2:

Overall probability: 0.486

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU91	0.43	0.86
GLU92	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
E91HA	1.00
E91HB3	1.00
E91HG2	1.00
E91HG3	1.00
E91H	1.00
E91HE2	1.00
E91HB2	1.00
E92H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU91	HA	1.00	0.040	0.00	0.00
GLU91	HB2	1.00	0.032	0.80	0.00
GLU91	HB3	1.00	0.032	0.80	0.00
GLU91	HG2	1.00	1.095	0.00	0.00
GLU91	HG3	1.00	2.449	0.00	0.00
GLU91	H	1.00	0.022	1.00	-1483442.00
GLU92	H	1.00	0.032	0.80	0.00

3.91.7 Detailed Probabilities of GLU91HB3:

Overall probability: 0.700

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU91	0.60	0.86
GLU92	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E91HA	1.00
E91HB2	1.00
E91HG2	1.00
E91HG3	1.00
E91H	1.00
E91HE2	1.00
E91HB3	1.00
E92H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU91	HA	1.00	0.009	1.00	5.05
GLU91	HB2	1.00	0.024	1.00	35.26
GLU91	HB3	1.00	0.024	1.00	35.26
GLU91	HG2	1.00	1.151	0.00	0.00
GLU91	HG3	1.00	2.505	0.00	0.00
GLU91	H	1.00	0.034	0.60	0.00
GLU92	H	1.00	0.024	1.00	-1706148.00
GLU92	HA	0.81	0.009	1.00	5.05

3.91.8 Detailed Probabilities of GLU91HG2:

Overall probability: 0.574

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU91	0.67	0.86
GLU92	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
E91HA	1.00
E91HB2	1.00
E91HB3	1.00
E91HG3	1.00
E91H	1.00
E91HE2	1.00
E91HG2	1.00
E92H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU91	HA	1.00	0.007	1.00	1.54
GLU91	HB2	1.00	0.013	1.00	2.04
GLU91	HB3	1.00	0.013	1.00	2.04
GLU91	HG2	1.00	0.803	0.00	0.00
GLU91	HG3	1.00	2.157	0.00	0.00
GLU91	H	1.00	0.000	1.00	-393850.00
GLU92	H	0.98	0.135	0.02	0.00

3.91.9 Detailed Probabilities of GLU91HG3:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU91	0.67	0.86
GLU92	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E91HA	1.00
E91HB2	1.00
E91HB3	1.00
E91HG2	1.00
E91H	1.00
E91HE2	1.00
E91HG3	1.00
E92H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU91	HA	1.00	0.005	1.00	2.14
GLU91	HB2	1.00	0.007	1.00	3.87
GLU91	HB3	1.00	0.007	1.00	3.87
GLU91	HG2	1.00	0.933	0.00	0.00
GLU91	HG3	1.00	2.287	0.00	0.00
GLU91	H	1.00	0.000	1.00	-484603.00
GLU92	H	0.97	0.005	1.00	-670034.00

3.91.10 Detailed Probabilities of GLU91H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU90	1.00	1.00
GLU91	1.00	1.00
GLU92	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L90HA	1.00
L90HB2	1.00
L90HB3	1.00
L90HG	0.98
L90H	1.00
E91HA	1.00
E91HB2	1.00
E91HB3	1.00
E91HG2	1.00
E91HG3	1.00
E91H	1.00
E92H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU90	HA	1.00	0.006	1.00	0.22
LEU90	HB2	1.00	0.004	1.00	0.19
LEU90	HB3	1.00	0.006	1.00	0.16
LEU90	HG	0.98	0.001	1.00	0.11
LEU90	H	1.00	0.006	1.00	-673755.00
LEU90	HD11	0.51	0.004	1.00	0.26
LEU90	HD21	0.58	0.004	1.00	0.26
GLU91	HA	1.00	0.002	1.00	0.75
GLU91	HB2	1.00	0.004	1.00	1.51
GLU91	HB3	1.00	0.004	1.00	1.51
GLU91	HG2	1.00	0.007	1.00	0.29
GLU91	HG3	1.00	0.010	1.00	0.24
GLU91	H	1.00	0.004	1.00	-8035352.00
GLU92	H	1.00	0.005	1.00	-538897.00
GLU92	HA	0.88	0.002	1.00	0.75

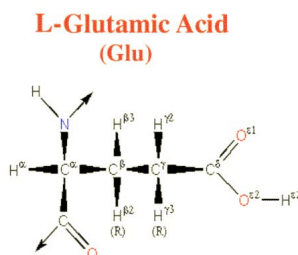


Figure 91: Image from the BMRB

Residue probability: 0.855
Residue probability confidence: 0.925

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.103	176.942	2.547	0.000	0.000
CA 3.92.1	59.252	57.442	3.837	0.864	1.000
CB 3.92.2	28.932	30.185	4.018	0.875	0.875
CG 3.92.3	36.010	36.085	1.533	0.986	0.875
N 3.92.4	118.667	120.574	4.837	0.815	1.000
HA 3.92.5	4.032	4.245	0.429	1.000	1.000
HB2 3.92.6	2.053	2.021	0.233	0.714	0.875
HB3 3.92.7	2.107	1.994	0.244	0.714	0.875
HG2 3.92.8	2.316	2.258	0.226	0.886	0.875
HG3 3.92.9	2.265	2.233	0.232	0.829	0.875
H 3.92.10	8.088	8.332	0.601	0.870	1.000
HE2	NA	—	—	0.000	0.000

3.92.1 Detailed Probabilities of GLU92CA:

Overall probability: 0.864
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU91	0.97	1.00
GLU92	0.93	1.00
PHE93	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E91HA	1.00
E92HB2	1.00
E92HB3	1.00
E92HG2	1.00
E92HG3	1.00
E92H	1.00
E92HA	1.00
F93H	1.00
F93HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU91	HA	1.00	0.031	0.90	0.00
GLU91	HB3	0.81	0.009	1.00	5.05
GLU91	H	0.88	0.002	1.00	0.75
GLU92	HA	1.00	0.010	1.00	41.95
GLU92	HB2	1.00	0.025	1.00	5.05
GLU92	HB3	1.00	0.029	1.00	5.05
GLU92	HG2	1.00	0.034	0.60	0.00
GLU92	HG3	1.00	0.017	1.00	2.14
GLU92	H	1.00	0.004	1.00	1.04
PHE93	HA	1.00	0.044	0.00	0.00
PHE93	H	1.00	0.011	1.00	1.04

3.92.2 Detailed Probabilities of GLU92CB:

Overall probability: 0.875

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU92	0.83	0.86
PHE93	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E92HA	1.00
E92HB2	1.00
E92HG2	1.00
E92HG3	1.00
E92H	1.00
E92HE2	1.00
E92HB3	1.00
F93H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU92	HA	1.00	0.004	1.00	2.70
GLU92	HB2	1.00	0.040	0.00	0.00
GLU92	HB3	1.00	0.014	1.00	35.26
GLU92	HG2	1.00	0.019	1.00	4.32
GLU92	HG3	1.00	0.015	1.00	3.87
GLU92	H	1.00	0.015	1.00	1.50
PHE93	H	1.00	0.000	1.00	1.50
PHE93	HA	0.85	0.007	1.00	0.59

3.92.3 Detailed Probabilities of GLU92CG:

Overall probability: 0.986

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU92	0.98	0.86
PHE93	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E92HA	1.00
E92HB2	1.00
E92HB3	1.00
E92HG3	1.00
E92H	1.00
E92HE2	1.00
E92HG2	1.00
F93H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU92	HA	1.00	0.005	1.00	2.08
GLU92	HB2	1.00	0.027	1.00	8.87
GLU92	HB3	1.00	0.027	1.00	8.87
GLU92	HG2	1.00	0.020	1.00	100.68
GLU92	HG3	1.00	0.031	0.90	0.00
GLU92	H	1.00	0.009	1.00	0.69
PHE93	H	0.99	0.006	1.00	0.69

3.92.4 Detailed Probabilities of GLU92N:

Overall probability: 0.815

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU91	0.80	1.00
GLU92	0.77	1.00
PHE93	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E91HG2	0.98
E91HA	1.00
E91H	1.00
E91HB3	1.00
E91HG3	0.97
E91HB2	1.00
E92HA	1.00
E92HB2	1.00
E92HB3	1.00
E92HG2	1.00
E92HG3	1.00
E92H	1.00
F93H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU91	HA	1.00	0.022	1.00	-909549.00
GLU91	HB2	1.00	0.032	0.80	0.00
GLU91	HB3	1.00	0.024	1.00	-1706148.00
GLU91	HG2	0.98	0.135	0.02	0.00
GLU91	HG3	0.97	0.005	1.00	-670034.00
GLU91	H	1.00	0.005	1.00	-538897.00
GLU92	HA	1.00	0.019	1.00	-909549.00
GLU92	HB2	1.00	0.040	0.00	0.00
GLU92	HB3	1.00	0.014	1.00	-1706148.00
GLU92	HG2	1.00	0.034	0.60	0.00
GLU92	HG3	1.00	0.017	1.00	-670034.00
GLU92	H	1.00	0.001	1.00	-8488027.00
PHE93	H	1.00	0.014	1.00	-8488027.00
PHE93	HA	0.93	0.001	1.00	-113678.00

3.92.5 Detailed Probabilities of GLU92HA:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU91	1.00	1.00
GLU92	1.00	1.00
PHE93	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E91HA	1.00
E92HB2	1.00
E92HB3	1.00
E92HG2	1.00
E92HG3	1.00
E92H	1.00
E92HA	1.00
F93H	1.00
F93HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU91	HA	1.00	0.010	1.00	41.95
GLU91	HB3	0.81	0.004	1.00	2.70
GLU92	HA	1.00	0.010	1.00	41.95
GLU92	HB2	1.00	0.004	1.00	2.70
GLU92	HB3	1.00	0.004	1.00	2.70
GLU92	HG2	1.00	0.005	1.00	2.08
GLU92	HG3	1.00	0.005	1.00	2.08
GLU92	H	1.00	0.019	1.00	-909549.00
PHE93	HA	1.00	0.021	1.00	2.23
PHE93	H	1.00	0.014	1.00	-290946.00

3.92.6 Detailed Probabilities of GLU92HB2:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU92	0.67	0.86
PHE93	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E92HA	1.00
E92HB3	1.00
E92HG2	1.00
E92HG3	1.00
E92H	1.00
E92HE2	1.00
E92HB2	1.00
F93H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU92	HA	1.00	0.025	1.00	5.05
GLU92	HB2	1.00	0.012	1.00	52.03
GLU92	HB3	1.00	0.040	0.00	0.00
GLU92	HG2	1.00	0.027	1.00	8.87
GLU92	HG3	1.00	0.027	1.00	8.87
GLU92	H	1.00	0.040	0.00	0.00
PHE93	H	1.00	0.020	1.00	-904565.00

3.92.7 Detailed Probabilities of GLU92HB3:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU92	0.83	0.86
PHE93	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E92HA	1.00
E92HB2	1.00
E92HG2	1.00
E92HG3	1.00
E92H	1.00
E92HE2	1.00
E92HB3	1.00
F93H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU92	HA	1.00	0.029	1.00	5.05
GLU92	HB2	1.00	0.228	0.00	0.00
GLU92	HB3	1.00	0.014	1.00	35.26
GLU92	HG2	1.00	0.027	1.00	8.87
GLU92	HG3	1.00	0.027	1.00	8.87
GLU92	H	1.00	0.014	1.00	-1706148.00
PHE93	H	1.00	0.074	0.00	0.00

3.92.8 Detailed Probabilities of GLU92HG2:

Overall probability: 0.886

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU92	0.87	0.86
PHE93	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E92HA	1.00
E92HB2	1.00
E92HB3	1.00
E92HG3	1.00
E92H	1.00
E92HE2	1.00
E92HG2	1.00
F93H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU92	HA	1.00	0.034	0.60	0.00
GLU92	HB2	1.00	0.019	1.00	4.32
GLU92	HB3	1.00	0.019	1.00	4.32
GLU92	HG2	1.00	0.020	1.00	100.68
GLU92	HG3	1.00	0.020	1.00	100.68
GLU92	H	1.00	0.034	0.60	0.00
PHE93	H	0.99	0.027	1.00	-193405.00

3.92.9 Detailed Probabilities of GLU92HG3:

Overall probability: 0.829

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU92	0.80	0.86
PHE93	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E92HA	1.00
E92HB2	1.00
E92HB3	1.00
E92HG2	1.00
E92H	1.00
E92HE2	1.00
E92HG3	1.00
F93H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU92	HA	1.00	0.017	1.00	2.14
GLU92	HB2	1.00	0.070	0.00	0.00
GLU92	HB3	1.00	0.015	1.00	3.87
GLU92	HG2	1.00	0.031	0.90	0.00
GLU92	HG3	1.00	0.031	0.90	0.00
GLU92	H	1.00	0.017	1.00	-670034.00
PHE93	H	0.98	0.024	1.00	-193405.00

3.92.10 Detailed Probabilities of GLU92H:

Overall probability: 0.870

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU91	0.67	1.00
GLU92	1.00	1.00
PHE93	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E91HG2	0.98
E91HA	1.00
E91H	1.00
E91HB3	1.00
E91HG3	0.97
E91HB2	1.00
E92HA	1.00
E92HB2	1.00
E92HB3	1.00
E92HG2	1.00
E92HG3	1.00
E92H	1.00
F93H	1.00

NOESY contacts detailed probability

3.92 GLU(92)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU91	HA	1.00	0.004	1.00	1.04
GLU91	HB2	1.00	0.015	1.00	1.50
GLU91	HB3	1.00	0.015	1.00	1.50
GLU91	HG2	0.98	0.141	0.02	0.00
GLU91	HG3	0.97	0.138	0.03	0.00
GLU91	H	1.00	0.009	1.00	-1240238.00
GLU92	HA	1.00	0.004	1.00	1.04
GLU92	HB2	1.00	0.008	1.00	1.37
GLU92	HB3	1.00	0.015	1.00	1.50
GLU92	HG2	1.00	0.009	1.00	0.69
GLU92	HG3	1.00	0.008	1.00	0.53
GLU92	H	1.00	0.001	1.00	-8488027.00
PHE93	H	1.00	0.025	1.00	-16420475.00
PHE93	HA	0.93	0.021	1.00	1.34
PHE93	HB2	0.59	0.020	1.00	0.71

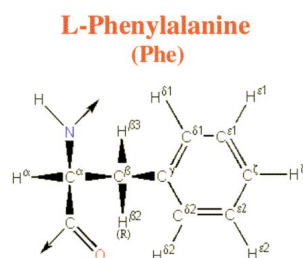
3.93 PHE(93)

Figure 92: Image from the BMRB

Residue probability: 0.664

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	176.894	175.508	2.010	0.000	0.000
CA 3.93.1	60.445	58.245	3.808	0.800	1.000
CB 3.93.2	38.987	40.078	3.616	1.000	1.000
CD1 3.93.3	131.517	131.234	9.579	0.556	1.000
CD2 3.93.4	131.641	131.352	9.581	0.557	1.000
CE1 3.93.5	130.552	130.599	3.219	0.600	1.000
CE2 3.93.6	130.600	130.633	2.839	0.429	1.000
CZ 3.93.7	129.169	129.042	3.448	0.200	1.000
N 3.93.8	120.118	120.315	4.931	0.929	1.000
HA 3.93.9	4.340	4.625	1.237	0.750	1.000
HB2 3.93.10	3.295	2.980	0.399	0.875	1.000
HB3 3.93.11	3.036	2.916	0.434	0.889	1.000
HD1 3.93.12	7.221	7.037	0.347	0.667	1.000
HD2 3.93.13	7.221	7.022	0.417	0.667	1.000
HE1 3.93.14	7.136	7.046	0.417	0.500	1.000
HE2 3.93.15	7.136	7.043	0.400	0.429	1.000
HZ 3.93.16	7.083	6.984	1.598	0.600	1.000
H 3.93.17	8.103	8.375	0.710	0.847	1.000

3.93.1 Detailed Probabilities of PHE93CA:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU92	1.00	1.00
PHE93	0.83	1.00
LYS94	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E92HA	1.00
F93HB2	1.00
F93HB3	1.00
F93HD1	1.00
F93HD2	1.00
F93H	1.00
F93HA	1.00
K94HA	1.00
K94H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU92	HA	1.00	0.021	1.00	2.23
GLU92	H	0.93	0.021	1.00	1.34
PHE93	HA	1.00	0.154	0.00	0.00
PHE93	HB2	1.00	0.002	1.00	0.65
PHE93	HB3	1.00	0.002	1.00	0.46
PHE93	HD1	1.00	0.001	1.00	0.68
PHE93	HD2	1.00	0.001	1.00	0.68
PHE93	H	1.00	0.006	1.00	1.34
LYS94	HA	1.00	0.189	0.00	0.00
LYS94	H	1.00	0.017	1.00	0.12

3.93.2 Detailed Probabilities of PHE93CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE93	1.00	1.00
LYS94	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F93HA	1.00
F93HB2	1.00
F93HD1	1.00
F93HD2	1.00
F93HE2	1.00
F93H	1.00
F93HB3	1.00
K94H	1.00

NOESY contacts detailed probability

3.93 PHE(93)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE93	HA	1.00	0.002	1.00	0.45
PHE93	HB2	1.00	0.002	1.00	1.51
PHE93	HB3	1.00	0.016	1.00	4.05
PHE93	HD1	1.00	0.005	1.00	0.40
PHE93	HD2	1.00	0.005	1.00	0.40
PHE93	HE2	1.00	0.003	1.00	0.43
PHE93	H	1.00	0.004	1.00	0.58
PHE93	HE1	0.89	0.003	1.00	0.43
LYS94	H	1.00	0.001	1.00	0.26

3.93.3 Detailed Probabilities of PHE93CD1:

Overall probability: 0.556

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE93	0.56	1.00

Expected NOESY Contacts

Proton	Expected probability
F93HA	1.00
F93HB2	1.00
F93HB3	1.00
F93HD2	1.00
F93HE1	1.00
F93HE2	1.00
F93HZ	1.00
F93H	1.00
F93HD1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE93	HA	1.00	0.011	1.00	0.43
PHE93	HB2	1.00	0.002	1.00	0.28
PHE93	HB3	1.00	0.002	1.00	0.45
PHE93	HD1	1.00	0.003	1.00	9.97
PHE93	HD2	1.00	0.003	1.00	9.97
PHE93	HE1	1.00	0.088	0.00	0.00
PHE93	HE2	1.00	0.088	0.00	0.00
PHE93	HZ	1.00	0.141	0.00	0.00
PHE93	H	1.00	0.879	0.00	0.00

3.93.4 Detailed Probabilities of PHE93CD2:

Overall probability: 0.557

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE93	0.56	1.00

Expected NOESY Contacts

Proton	Expected probability
F93HA	1.00
F93HB2	1.00
F93HB3	1.00
F93HD1	1.00
F93HE1	1.00
F93HE2	1.00
F93HZ	1.00
F93H	0.99
F93HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE93	HA	1.00	0.011	1.00	0.43
PHE93	HB2	1.00	0.002	1.00	0.28
PHE93	HB3	1.00	0.002	1.00	0.45
PHE93	HD1	1.00	0.003	1.00	9.97
PHE93	HD2	1.00	0.003	1.00	9.97
PHE93	HE1	1.00	0.088	0.00	0.00
PHE93	HE2	1.00	0.088	0.00	0.00
PHE93	HZ	1.00	0.141	0.00	0.00
PHE93	H	0.99	0.879	0.01	0.00

3.93.5 Detailed Probabilities of PHE93CE1:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE93	0.60	1.00

Expected NOESY Contacts

Proton	Expected probability
F93HD1	1.00
F93HD2	1.00
F93HE2	1.00
F93HZ	1.00
F93HE1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE93	HD1	1.00	0.115	0.00	0.00
PHE93	HD2	1.00	0.115	0.00	0.00
PHE93	HE1	1.00	0.030	1.00	0.00
PHE93	HE2	1.00	0.030	1.00	0.00
PHE93	HZ	1.00	0.023	1.00	15.02

3.93.6 Detailed Probabilities of PHE93CE2:

Overall probability: 0.429

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE93	0.43	1.00

Expected NOESY Contacts

Proton	Expected probability
F93HB2	1.00
F93HB3	1.00
F93HD1	1.00
F93HD2	1.00
F93HE1	1.00
F93HZ	1.00
F93HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE93	HB2	1.00	2.265	0.00	0.00
PHE93	HB3	1.00	2.524	0.00	0.00
PHE93	HD1	1.00	0.115	0.00	0.00
PHE93	HD2	1.00	0.115	0.00	0.00
PHE93	HE1	1.00	0.030	1.00	0.00
PHE93	HE2	1.00	0.030	1.00	0.00
PHE93	HZ	1.00	0.023	1.00	15.02

3.93.7 Detailed Probabilities of PHE93CZ:

Overall probability: 0.200

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE93	0.20	1.00

Expected NOESY Contacts

Proton	Expected probability
F93HD1	1.00
F93HD2	1.00
F93HE1	1.00
F93HE2	1.00
F93HZ	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE93	HD1	1.00	0.136	0.00	0.00
PHE93	HD2	1.00	0.136	0.00	0.00
PHE93	HE1	1.00	0.051	0.00	0.00
PHE93	HE2	1.00	0.051	0.00	0.00
PHE93	HZ	1.00	0.002	1.00	12.46

3.93.8 Detailed Probabilities of PHE93N:

Overall probability: 0.929

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU92	0.83	1.00
PHE93	1.00	1.00
LYS94	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E92HB3	1.00
E92HG3	0.98
E92HG2	0.99
E92HA	1.00
E92H	1.00
E92HB2	1.00
F93HA	1.00
F93HB2	1.00
F93HB3	1.00
F93HD1	1.00
F93HD2	0.99
F93H	1.00
K94H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU92	HA	1.00	0.014	1.00	-290946.00
GLU92	HB2	1.00	0.020	1.00	-904565.00
GLU92	HB3	1.00	0.074	0.00	0.00
GLU92	HG2	0.99	0.027	1.00	-193405.00
GLU92	HG3	0.98	0.024	1.00	-193405.00
GLU92	H	1.00	0.025	1.00	-16420475.00
PHE93	HA	1.00	0.001	1.00	-776158.00
PHE93	HB2	1.00	0.005	1.00	-1479803.00
PHE93	HB3	1.00	0.002	1.00	-1080422.00
PHE93	HD1	1.00	0.003	1.00	-289197.00
PHE93	HD2	0.99	0.003	1.00	-289197.00
PHE93	H	1.00	0.010	1.00	-16420475.00
LYS94	H	1.00	0.001	1.00	-894047.00
LYS94	HB2	0.51	0.015	1.00	-2103946.00

3.93.9 Detailed Probabilities of PHE93HA:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU92	0.75	1.00
PHE93	0.83	1.00
LYS94	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E92HA	1.00
F93HB2	1.00
F93HB3	1.00
F93HD1	1.00
F93HD2	1.00
F93H	1.00
F93HA	1.00
K94HA	1.00
K94H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU92	HA	1.00	0.044	0.00	0.00
GLU92	HB2	0.71	0.007	1.00	0.59
GLU92	HB3	0.85	0.007	1.00	0.59
GLU92	H	0.93	0.001	1.00	-113678.00
PHE93	HA	1.00	0.154	0.00	0.00
PHE93	HB2	1.00	0.001	1.00	0.51
PHE93	HB3	1.00	0.002	1.00	0.45
PHE93	HD1	1.00	0.011	1.00	0.43
PHE93	HD2	1.00	0.011	1.00	0.43
PHE93	H	1.00	0.001	1.00	-776158.00
LYS94	HA	1.00	0.392	0.00	0.00
LYS94	H	1.00	0.002	1.00	-220806.00

3.93.10 Detailed Probabilities of PHE93HB2:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE93	0.86	1.00
LYS94	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F93HA	1.00
F93HB3	1.00
F93HD1	1.00
F93HD2	1.00
F93HE2	1.00
F93H	1.00
F93HB2	1.00
K94H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE93	HA	1.00	0.002	1.00	0.65
PHE93	HB2	1.00	0.003	1.00	1.88
PHE93	HB3	1.00	0.002	1.00	1.51
PHE93	HD1	1.00	0.002	1.00	0.28
PHE93	HD2	1.00	0.002	1.00	0.28
PHE93	HE2	1.00	2.265	0.00	0.00
PHE93	H	1.00	0.005	1.00	-1479803.00
LYS94	H	1.00	0.005	1.00	-361012.00

3.93.11 Detailed Probabilities of PHE93HB3:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE93	0.86	1.00
LYS94	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F93HA	1.00
F93HB2	1.00
F93HD1	1.00
F93HD2	1.00
F93HE2	1.00
F93H	1.00
F93HB3	1.00
K94H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE93	HA	1.00	0.002	1.00	0.46
PHE93	HB2	1.00	0.000	1.00	1.51
PHE93	HB3	1.00	0.016	1.00	4.05
PHE93	HD1	1.00	0.002	1.00	0.45
PHE93	HD2	1.00	0.002	1.00	0.45
PHE93	HE2	1.00	2.524	0.00	0.00
PHE93	H	1.00	0.002	1.00	-1080422.00
LYS94	H	1.00	0.003	1.00	-549294.00
LYS94	HA	0.86	0.014	1.00	0.06

3.93.12 Detailed Probabilities of PHE93HD1:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE93	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
F93HA	1.00
F93HB2	1.00
F93HB3	1.00
F93HD2	1.00
F93HE1	1.00
F93HE2	1.00
F93HZ	1.00
F93H	1.00
F93HD1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE93	HA	1.00	0.001	1.00	0.68
PHE93	HB2	1.00	0.004	1.00	0.41
PHE93	HB3	1.00	0.005	1.00	0.40
PHE93	HD1	1.00	0.003	1.00	9.97
PHE93	HD2	1.00	0.003	1.00	9.97
PHE93	HE1	1.00	0.115	0.00	0.00
PHE93	HE2	1.00	0.115	0.00	0.00
PHE93	HZ	1.00	0.136	0.00	0.00
PHE93	H	1.00	0.003	1.00	-289197.00

3.93.13 Detailed Probabilities of PHE93HD2:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE93	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
F93HA	1.00
F93HB2	1.00
F93HB3	1.00
F93HD1	1.00
F93HE1	1.00
F93HE2	1.00
F93HZ	1.00
F93H	0.99
F93HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE93	HA	1.00	0.001	1.00	0.68
PHE93	HB2	1.00	0.004	1.00	0.41
PHE93	HB3	1.00	0.005	1.00	0.40
PHE93	HD1	1.00	0.003	1.00	9.97
PHE93	HD2	1.00	0.003	1.00	9.97
PHE93	HE1	1.00	0.115	0.00	0.00
PHE93	HE2	1.00	0.115	0.00	0.00
PHE93	HZ	1.00	0.136	0.00	0.00
PHE93	H	0.99	0.003	1.00	-289197.00

3.93.14 Detailed Probabilities of PHE93HE1:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE93	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
F93HD1	1.00
F93HD2	1.00
F93HE2	1.00
F93HZ	1.00
F93HE1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE93	HD1	1.00	0.088	0.00	0.00
PHE93	HD2	1.00	0.088	0.00	0.00
PHE93	HE1	1.00	0.030	1.00	0.00
PHE93	HE2	1.00	0.030	1.00	0.00
PHE93	HZ	1.00	0.051	0.00	0.00
PHE93	HB3	0.89	0.003	1.00	0.43

3.93.15 Detailed Probabilities of PHE93HE2:

Overall probability: 0.429

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE93	0.43	1.00

Expected NOESY Contacts

Proton	Expected probability
F93HB2	1.00
F93HB3	1.00
F93HD1	1.00
F93HD2	1.00
F93HE1	1.00
F93HZ	1.00
F93HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE93	HB2	1.00	0.089	0.00	0.00
PHE93	HB3	1.00	0.003	1.00	0.43
PHE93	HD1	1.00	0.088	0.00	0.00
PHE93	HD2	1.00	0.088	0.00	0.00
PHE93	HE1	1.00	0.030	1.00	0.00
PHE93	HE2	1.00	0.030	1.00	0.00
PHE93	HZ	1.00	0.051	0.00	0.00

3.93.16 Detailed Probabilities of PHE93HZ:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE93	0.60	1.00

Expected NOESY Contacts

Proton	Expected probability
F93HD1	1.00
F93HD2	1.00
F93HE1	1.00
F93HE2	1.00
F93HZ	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE93	HD1	1.00	0.141	0.00	0.00
PHE93	HD2	1.00	0.141	0.00	0.00
PHE93	HE1	1.00	0.023	1.00	15.02
PHE93	HE2	1.00	0.023	1.00	15.02
PHE93	HZ	1.00	0.002	1.00	12.46

3.93.17 Detailed Probabilities of PHE93H:

Overall probability: 0.847

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU92	1.00	1.00
PHE93	0.67	1.00
LYS94	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E92HB3	1.00
E92HG3	0.98
E92HG2	0.99
E92HA	1.00
E92H	1.00
E92HB2	1.00
F93HA	1.00
F93HB2	1.00
F93HB3	1.00
F93HD1	1.00
F93HD2	0.99
F93H	1.00
K94H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU92	HA	1.00	0.011	1.00	1.04
GLU92	HB2	1.00	0.007	1.00	1.37
GLU92	HB3	1.00	0.000	1.00	1.50
GLU92	HG2	0.99	0.006	1.00	0.69
GLU92	HG3	0.98	0.006	1.00	0.69
GLU92	H	1.00	0.014	1.00	-8488027.00
PHE93	HA	1.00	0.006	1.00	1.34
PHE93	HB2	1.00	0.005	1.00	0.71
PHE93	HB3	1.00	0.004	1.00	0.58
PHE93	HD1	1.00	0.879	0.00	0.00
PHE93	HD2	0.99	0.879	0.01	0.00
PHE93	H	1.00	0.010	1.00	-16420475.00
LYS94	H	1.00	0.013	1.00	-936204.00

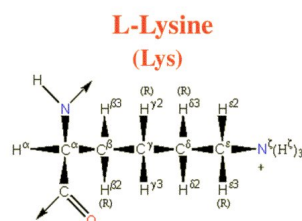


Figure 93: Image from the BMRB

Residue probability: 0.699
Residue probability confidence: 0.941

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	177.600	176.660	3.133	0.000	0.000
CA 3.94.1	60.076	57.014	3.028	0.773	1.000
CB 3.94.2	32.465	32.981	3.186	0.800	1.000
CG 3.94.3	24.715	24.941	1.956	0.778	0.900
CD 3.94.4	30.102	29.020	2.193	0.180	0.889
CE 3.94.5	41.780	41.893	1.492	0.763	0.875
N 3.94.6	118.941	120.954	4.210	0.900	1.000
NZ	NA	—	—	0.000	0.000
HA 3.94.7	3.617	4.262	0.489	0.835	1.000
HB2 3.94.8	2.070	1.774	0.365	0.740	1.000
HB3 3.94.9	1.735	1.742	0.385	0.381	1.000
HG2 3.94.10	1.369	1.358	0.344	0.610	0.909
HG3 3.94.11	1.321	1.343	0.357	0.667	0.900
HD 3.94.12	1.537	1.614	0.957	0.667	0.889
HE2 3.94.13	3.019	2.907	0.230	0.738	0.875
HE3 3.94.14	2.917	2.901	0.241	0.659	0.875
H 3.94.15	8.606	8.185	0.605	1.000	1.000
HZ	NA	—	—	0.000	0.000

3.94.1 Detailed Probabilities of LYS94CA:

Overall probability: 0.773
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE93	0.50	1.00
LYS94	0.93	1.00
ARG95	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
F93HA	1.00
K94HB2	1.00
K94HB3	1.00
K94HG2	1.00
K94HG3	1.00
K94HD2	0.98
K94H	1.00
K94HA	1.00
R95HA	1.00
R95H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE93	HA	1.00	0.392	0.00	0.00
PHE93	HB3	0.86	0.014	1.00	0.06
LYS94	HA	1.00	0.005	1.00	5.04
LYS94	HB2	1.00	0.004	1.00	0.47
LYS94	HB3	1.00	0.008	1.00	0.67
LYS94	HG2	1.00	0.035	0.50	0.00
LYS94	HG3	1.00	0.013	1.00	0.59
LYS94	HD2	0.98	0.012	1.00	0.17
LYS94	H	1.00	0.001	1.00	0.51
ARG95	HA	1.00	0.202	0.00	0.00
ARG95	H	1.00	0.009	1.00	0.17

3.94.2 Detailed Probabilities of LYS94CB:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS94	0.78	1.00
ARG95	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K94HA	1.00
K94HB3	1.00
K94HG2	1.00
K94HG3	1.00
K94HD2	1.00
K94HE2	0.98
K94HE3	0.99
K94H	1.00
K94HB2	1.00
R95H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS94	HA	1.00	0.005	1.00	0.25
LYS94	HB2	1.00	0.333	0.00	0.00
LYS94	HB3	1.00	0.002	1.00	1.40
LYS94	HG2	1.00	0.018	1.00	0.39
LYS94	HG3	1.00	0.030	1.00	0.00
LYS94	HD2	1.00	0.186	0.00	0.00
LYS94	HE2	0.98	0.008	1.00	0.09
LYS94	HE3	0.99	0.010	1.00	0.07
LYS94	H	1.00	0.000	1.00	0.39
ARG95	H	1.00	0.007	1.00	0.26

3.94.3 Detailed Probabilities of LYS94CG:

Overall probability: 0.778

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS94	0.78	0.90

Expected NOESY Contacts

Proton	Expected probability
K94HA	1.00
K94HB2	1.00
K94HB3	1.00
K94HG2	1.00
K94HD2	1.00
K94HE2	1.00
K94HE3	1.00
K94H	1.00
K94HZ2	1.00
K94HG3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS94	HA	1.00	0.005	1.00	0.25
LYS94	HB2	1.00	0.007	1.00	0.44
LYS94	HB3	1.00	0.124	0.00	0.00
LYS94	HG2	1.00	0.187	0.00	0.00
LYS94	HG3	1.00	0.019	1.00	15.45
LYS94	HD2	1.00	0.021	1.00	5.34
LYS94	HE2	1.00	0.023	1.00	0.12
LYS94	HE3	1.00	0.003	1.00	0.63
LYS94	H	1.00	0.004	1.00	0.17

3.94.4 Detailed Probabilities of LYS94CD:

Overall probability: 0.180

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS94	0.18	0.89

Expected NOESY Contacts

Proton	Expected probability
K94HA	0.98
K94HB2	1.00
K94HB3	1.00
K94HG2	1.00
K94HG3	1.00
K94HD3	1.00
K94HE2	1.00
K94HE3	1.00
K94HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS94	HA	0.98	0.380	0.02	0.00
LYS94	HB2	1.00	0.122	0.00	0.00
LYS94	HB3	1.00	0.213	0.00	0.00
LYS94	HG2	1.00	0.046	0.00	0.00
LYS94	HG3	1.00	0.094	0.00	0.00
LYS94	HD2	1.00	0.122	0.00	0.00
LYS94	HE2	1.00	0.136	0.00	0.00
LYS94	HE3	1.00	0.034	0.60	0.00
LYS94	H	0.87	0.003	1.00	0.11

3.94.5 Detailed Probabilities of LYS94CE:

Overall probability: 0.763

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS94	0.76	0.88

Expected NOESY Contacts

Proton	Expected probability
K94HB2	0.98
K94HB3	0.99
K94HG2	1.00
K94HG3	1.00
K94HD2	1.00
K94HE3	1.00
K94HZ2	1.00
K94HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS94	HB2	0.98	0.005	1.00	0.54
LYS94	HB3	0.99	0.039	0.10	0.00
LYS94	HG2	1.00	0.006	1.00	0.43
LYS94	HG3	1.00	0.144	0.00	0.00
LYS94	HD2	1.00	0.030	1.00	0.00
LYS94	HE2	1.00	0.011	1.00	227.40
LYS94	HE3	1.00	0.004	1.00	5.24
LYS94	HA	0.77	0.015	1.00	0.11

3.94.6 Detailed Probabilities of LYS94N:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE93	1.00	1.00
LYS94	0.94	1.00
ARG95	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F93HB2	1.00
F93HB3	1.00
F93HA	1.00
F93H	1.00
K94HA	1.00
K94HB2	1.00
K94HB3	1.00
K94HG2	1.00
K94HG3	1.00
K94H	1.00
R95H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE93	HA	1.00	0.002	1.00	-220806.00
PHE93	HB2	1.00	0.005	1.00	-361012.00
PHE93	HB3	1.00	0.003	1.00	-549294.00
PHE93	H	1.00	0.013	1.00	-936204.00
PHE93	HD1	0.78	0.003	1.00	-179600.00
PHE93	HD2	0.64	0.003	1.00	-179600.00
LYS94	HA	1.00	0.003	1.00	-725648.00
LYS94	HB2	1.00	0.005	1.00	-1060425.00
LYS94	HB3	1.00	0.001	1.00	-1023298.00
LYS94	HG2	1.00	0.034	0.60	0.00
LYS94	HG3	1.00	0.014	1.00	-317997.00
LYS94	H	1.00	0.001	1.00	-6519571.00
LYS94	HD2	0.88	0.016	1.00	-166156.00
ARG95	H	1.00	0.043	0.00	0.00

3.94.7 Detailed Probabilities of LYS94HA:

Overall probability: 0.835

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE93	0.00	1.00
LYS94	0.89	1.00
ARG95	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F93HA	1.00
K94HB2	1.00
K94HB3	1.00
K94HG2	1.00
K94HG3	1.00
K94HD2	0.98
K94H	1.00
K94HA	1.00
R95HA	1.00
R95H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE93	HA	1.00	0.189	0.00	0.00
LYS94	HA	1.00	0.005	1.00	5.04
LYS94	HB2	1.00	0.005	1.00	0.25
LYS94	HB3	1.00	0.007	1.00	0.33
LYS94	HG2	1.00	0.005	1.00	0.25
LYS94	HG3	1.00	0.005	1.00	0.25
LYS94	HD2	0.98	0.380	0.02	0.00
LYS94	H	1.00	0.003	1.00	-725648.00
LYS94	HE2	0.77	0.015	1.00	0.11
LYS94	HE3	0.76	0.014	1.00	0.06
ARG95	HA	1.00	0.003	1.00	0.05
ARG95	H	1.00	0.007	1.00	-299660.00

3.94.8 Detailed Probabilities of LYS94HB2:

Overall probability: 0.740

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS94	0.71	1.00
ARG95	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K94HA	1.00
K94HB3	1.00
K94HG2	1.00
K94HG3	1.00
K94HD2	1.00
K94HE2	0.98
K94HE3	0.99
K94H	1.00
K94HB2	1.00
R95H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS94	HA	1.00	0.004	1.00	0.47
LYS94	HB2	1.00	0.333	0.00	0.00
LYS94	HB3	1.00	0.005	1.00	1.19
LYS94	HG2	1.00	0.007	1.00	0.44
LYS94	HG3	1.00	0.007	1.00	0.44
LYS94	HD2	1.00	0.122	0.00	0.00
LYS94	HE2	0.98	0.005	1.00	0.54
LYS94	HE3	0.99	0.036	0.40	0.00
LYS94	H	1.00	0.005	1.00	-1060425.00
ARG95	H	1.00	0.004	1.00	-667336.00

3.94.9 Detailed Probabilities of LYS94HB3:

Overall probability: 0.381

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS94	0.42	1.00
ARG95	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K94HA	1.00
K94HB2	1.00
K94HG2	1.00
K94HG3	1.00
K94HD2	1.00
K94HE2	0.99
K94HE3	0.99
K94H	1.00
K94HB3	1.00
R95H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS94	HA	1.00	0.008	1.00	0.67
LYS94	HB2	1.00	0.002	1.00	1.40
LYS94	HB3	1.00	0.033	0.70	0.00
LYS94	HG2	1.00	0.100	0.00	0.00
LYS94	HG3	1.00	0.124	0.00	0.00
LYS94	HD2	1.00	0.213	0.00	0.00
LYS94	HE2	0.99	0.039	0.10	0.00
LYS94	HE3	0.99	0.071	0.01	0.00
LYS94	H	1.00	0.001	1.00	-1023298.00
ARG95	H	1.00	0.046	0.00	0.00

3.94.10 Detailed Probabilities of LYS94HG2:

Overall probability: 0.610

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS94	0.57	0.90
ARG95	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K94HA	1.00
K94HB2	1.00
K94HB3	1.00
K94HG3	1.00
K94HD2	1.00
K94HE2	1.00
K94HE3	1.00
K94H	1.00
K94HZ2	1.00
K94HG2	1.00
R95H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS94	HA	1.00	0.035	0.50	0.00
LYS94	HB2	1.00	0.018	1.00	0.39
LYS94	HB3	1.00	0.025	1.00	0.46
LYS94	HG2	1.00	0.015	1.00	36.93
LYS94	HG3	1.00	0.187	0.00	0.00
LYS94	HD2	1.00	0.046	0.00	0.00
LYS94	HE2	1.00	0.006	1.00	0.43
LYS94	HE3	1.00	0.042	0.00	0.00
LYS94	H	1.00	0.034	0.60	0.00
ARG95	H	0.96	0.028	1.00	-177293.00

3.94.11 Detailed Probabilities of LYS94HG3:

Overall probability: 0.667

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS94	0.67	0.90

Expected NOESY Contacts

Proton	Expected probability
K94HA	1.00
K94HB2	1.00
K94HB3	1.00
K94HG2	1.00
K94HD2	1.00
K94HE2	1.00
K94HE3	1.00
K94H	1.00
K94HZ2	1.00
K94HG3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS94	HA	1.00	0.013	1.00	0.59
LYS94	HB2	1.00	0.030	1.00	0.00
LYS94	HB3	1.00	0.023	1.00	0.46
LYS94	HG2	1.00	0.063	0.00	0.00
LYS94	HG3	1.00	0.019	1.00	15.45
LYS94	HD2	1.00	0.094	0.00	0.00
LYS94	HE2	1.00	0.144	0.00	0.00
LYS94	HE3	1.00	0.012	1.00	0.77
LYS94	H	1.00	0.014	1.00	-317997.00

3.94.12 Detailed Probabilities of LYS94HD2:

Overall probability: 0.667

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS94	0.67	0.89

Expected NOESY Contacts

Proton	Expected probability
K94HA	0.98
K94HB2	1.00
K94HB3	1.00
K94HG2	1.00
K94HG3	1.00
K94HD3	1.00
K94HE2	1.00
K94HE3	1.00
K94HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS94	HA	0.98	0.012	1.00	0.17
LYS94	HB2	1.00	0.186	0.00	0.00
LYS94	HB3	1.00	0.070	0.00	0.00
LYS94	HG2	1.00	0.005	1.00	4.89
LYS94	HG3	1.00	0.021	1.00	5.34
LYS94	HD2	1.00	0.122	0.00	0.00
LYS94	HE2	1.00	0.030	1.00	0.00
LYS94	HE3	1.00	0.023	1.00	1.96
LYS94	H	0.87	0.016	1.00	-166156.00

3.94.13 Detailed Probabilities of LYS94HE2:

Overall probability: 0.738

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS94	0.74	0.88

Expected NOESY Contacts

Proton	Expected probability
K94HB2	0.98
K94HB3	0.99
K94HG2	1.00
K94HG3	1.00
K94HD2	1.00
K94HE3	1.00
K94HZ2	1.00
K94HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS94	HB2	0.98	0.008	1.00	0.09
LYS94	HB3	0.99	0.004	1.00	0.12
LYS94	HG2	1.00	0.045	0.00	0.00
LYS94	HG3	1.00	0.023	1.00	0.12
LYS94	HD2	1.00	0.136	0.00	0.00
LYS94	HE2	1.00	0.011	1.00	227.40
LYS94	HE3	1.00	0.023	1.00	5.55
LYS94	HA	0.77	0.031	0.90	0.00

3.94.14 Detailed Probabilities of LYS94HE3:

Overall probability: 0.659

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS94	0.66	0.88

Expected NOESY Contacts

Proton	Expected probability
K94HB2	0.99
K94HB3	0.99
K94HG2	1.00
K94HG3	1.00
K94HD2	1.00
K94HE2	1.00
K94HZ2	1.00
K94HE3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS94	HB2	0.99	0.010	1.00	0.07
LYS94	HB3	0.99	0.106	0.01	0.00
LYS94	HG2	1.00	0.049	0.00	0.00
LYS94	HG3	1.00	0.003	1.00	0.63
LYS94	HD2	1.00	0.034	0.60	0.00
LYS94	HE2	1.00	0.004	1.00	5.24
LYS94	HE3	1.00	0.000	1.00	220.78

3.94.15 Detailed Probabilities of LYS94H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE93	1.00	1.00
LYS94	1.00	1.00
ARG95	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F93HB2	1.00
F93HB3	1.00
F93HA	1.00
F93H	1.00
K94HA	1.00
K94HB2	1.00
K94HB3	1.00
K94HG2	1.00
K94HG3	1.00
K94H	1.00
R95H	1.00

NOESY contacts detailed probability

3.94 LYS(94)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE93	HA	1.00	0.017	1.00	0.12
PHE93	HB2	1.00	0.000	1.00	0.23
PHE93	HB3	1.00	0.001	1.00	0.26
PHE93	H	1.00	0.001	1.00	-894047.00
LYS94	HA	1.00	0.001	1.00	0.51
LYS94	HB2	1.00	0.000	1.00	0.39
LYS94	HB3	1.00	0.001	1.00	0.57
LYS94	HG2	1.00	0.004	1.00	0.17
LYS94	HG3	1.00	0.004	1.00	0.17
LYS94	H	1.00	0.001	1.00	-6519571.00
LYS94	HD2	0.88	0.003	1.00	0.11
ARG95	H	1.00	0.001	1.00	-650545.00
ARG95	HB2	0.59	0.012	1.00	0.08

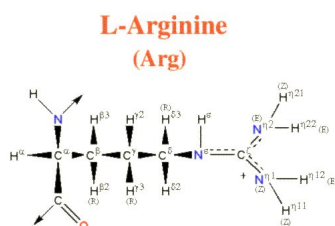


Figure 94: Image from the BMRB

Residue probability: 0.658
 Residue probability confidence: 0.864

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	179.404	176.453	2.303	0.000	0.000
CA 3.95.1	59.103	56.803	3.326	0.636	1.000
CB 3.95.2	29.819	30.892	2.424	0.900	0.900
CG 3.95.3	27.310	27.247	1.538	0.559	0.818
CD 3.95.4	43.413	43.189	1.415	0.875	0.700
N 3.95.5	117.194	120.701	3.779	0.600	1.000
NE	NA	—	—	0.000	0.000
NH1	NA	—	—	0.000	0.000
NH2	NA	—	—	0.000	0.000
HA 3.95.6	4.150	4.301	0.495	0.545	1.000
HB2 3.95.7	1.897	1.793	0.292	0.500	0.900
HB3 3.95.8	1.970	1.757	0.307	0.222	0.900
HG2 3.95.9	1.876	1.559	0.294	0.448	0.818
HG3 3.95.10	1.675	1.535	0.310	0.750	0.800
HD2 3.95.11	3.222	3.105	0.301	0.875	0.700
HD3 3.95.12	3.223	3.081	0.306	0.875	0.700
H 3.95.13	8.159	8.248	0.623	0.765	1.000
HE	NA	—	—	0.000	0.000
HH1	NA	—	—	0.000	0.000
HH2	NA	—	—	0.000	0.000

3.95.1 Detailed Probabilities of ARG95CA:

Overall probability: 0.636
 Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS94	1.00	1.00
ARG95	0.63	1.00
LYS96	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K94HA	1.00
R95HB2	1.00
R95HB3	1.00
R95HG2	1.00
R95HG3	1.00
R95HD2	0.98
R95HD3	0.97
R95H	1.00
R95HA	1.00
K96HA	1.00
K96H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS94	HA	1.00	0.003	1.00	0.05
ARG95	HA	1.00	0.005	1.00	24.81
ARG95	HB2	1.00	0.136	0.00	0.00
ARG95	HB3	1.00	0.063	0.00	0.00
ARG95	HG2	1.00	0.157	0.00	0.00
ARG95	HG3	1.00	0.007	1.00	1.13
ARG95	HD2	0.98	0.010	1.00	0.25
ARG95	HD3	0.97	0.009	1.00	0.25
ARG95	H	1.00	0.007	1.00	0.78
LYS96	HA	1.00	0.080	0.00	0.00
LYS96	H	1.00	0.011	1.00	0.30

3.95.2 Detailed Probabilities of ARG95CB:

Overall probability: 0.900

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG95	0.88	0.89
LYS96	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R95HA	1.00
R95HB3	1.00
R95HG2	1.00
R95HG3	1.00
R95HD2	1.00
R95HD3	1.00
R95H	1.00
R95HE	1.00
R95HB2	1.00
K96H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG95	HA	1.00	0.002	1.00	0.91
ARG95	HB2	1.00	0.007	1.00	14.73
ARG95	HB3	1.00	0.066	0.00	0.00
ARG95	HG2	1.00	0.028	1.00	14.73
ARG95	HG3	1.00	0.013	1.00	1.08
ARG95	HD2	1.00	0.001	1.00	0.62
ARG95	HD3	1.00	0.002	1.00	0.62
ARG95	H	1.00	0.007	1.00	0.65
LYS96	H	1.00	0.004	1.00	0.26
LYS96	HA	0.66	0.023	1.00	0.54

3.95.3 Detailed Probabilities of ARG95CG:

Overall probability: 0.559

Overall confidence: 0.818

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG95	0.63	0.80
LYS96	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
R95HA	1.00
R95HB2	1.00
R95HB3	1.00
R95HG3	1.00
R95HD2	1.00
R95HD3	1.00
R95H	1.00
R95HE	1.00
R95HH11	1.00
R95HG2	1.00
K96H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG95	HA	1.00	0.001	1.00	0.52
ARG95	HB2	1.00	0.026	1.00	12.24
ARG95	HB3	1.00	0.099	0.00	0.00
ARG95	HG2	1.00	0.005	1.00	12.24
ARG95	HG3	1.00	0.196	0.00	0.00
ARG95	HD2	1.00	0.000	1.00	0.89
ARG95	HD3	1.00	0.001	1.00	0.89
ARG95	H	1.00	0.097	0.00	0.00
LYS96	H	0.97	0.276	0.03	0.00

3.95.4 Detailed Probabilities of ARG95CD:

Overall probability: 0.875

Overall confidence: 0.700

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG95	0.88	0.70

Expected NOESY Contacts

Proton	Expected probability
R95HA	0.98
R95HB2	1.00
R95HB3	1.00
R95HG2	1.00
R95HG3	1.00
R95HD3	1.00
R95HE	1.00
R95HH11	1.00
R95HH21	1.00
R95HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG95	HA	0.97	0.005	1.00	0.21
ARG95	HB2	1.00	0.008	1.00	1.40
ARG95	HB3	1.00	0.081	0.00	0.00
ARG95	HG2	1.00	0.013	1.00	1.40
ARG95	HG3	1.00	0.002	1.00	1.17
ARG95	HD2	1.00	0.001	1.00	28.04
ARG95	HD3	1.00	0.002	1.00	28.04
ARG95	H	0.86	0.005	1.00	0.12

3.95.5 Detailed Probabilities of ARG95N:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS94	0.83	1.00
ARG95	0.38	1.00
LYS96	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K94HB3	1.00
K94H	1.00
K94HG2	0.96
K94HA	1.00
K94HB2	1.00
R95HA	1.00
R95HB2	1.00
R95HB3	1.00
R95HG2	1.00
R95HG3	1.00
R95H	1.00
K96H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS94	HA	1.00	0.007	1.00	-299660.00
LYS94	HB2	1.00	0.004	1.00	-667336.00
LYS94	HB3	1.00	0.046	0.00	0.00
LYS94	HG2	0.96	0.028	1.00	-177293.00
LYS94	H	1.00	0.001	1.00	-650545.00
LYS94	HG3	0.94	0.020	1.00	-177293.00
ARG95	HA	1.00	0.526	0.00	0.00
ARG95	HB2	1.00	0.169	0.00	0.00
ARG95	HB3	1.00	0.096	0.00	0.00
ARG95	HG2	1.00	0.187	0.00	0.00
ARG95	HG3	1.00	0.014	1.00	-597132.00
ARG95	H	1.00	0.114	0.00	0.00
ARG95	HD2	0.87	0.005	1.00	-134082.00
ARG95	HD3	0.86	0.004	1.00	-134082.00
LYS96	H	1.00	0.006	1.00	-859333.00

3.95.6 Detailed Probabilities of ARG95HA:

Overall probability: 0.545

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS94	0.00	1.00
ARG95	0.75	1.00
LYS96	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K94HA	1.00
R95HB2	1.00
R95HB3	1.00
R95HG2	1.00
R95HG3	1.00
R95HD2	0.98
R95HD3	0.97
R95H	1.00
R95HA	1.00
K96HA	1.00
K96H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS94	HA	1.00	0.202	0.00	0.00
ARG95	HA	1.00	0.005	1.00	24.81
ARG95	HB2	1.00	0.002	1.00	0.91
ARG95	HB3	1.00	0.006	1.00	0.99
ARG95	HG2	1.00	0.001	1.00	0.52
ARG95	HG3	1.00	0.131	0.00	0.00
ARG95	HD2	0.98	0.005	1.00	0.21
ARG95	HD3	0.97	0.005	1.00	0.21
ARG95	H	1.00	0.526	0.00	0.00
LYS96	HA	1.00	0.108	0.00	0.00
LYS96	H	1.00	0.078	0.00	0.00

3.95.7 Detailed Probabilities of ARG95HB2:

Overall probability: 0.500

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG95	0.50	0.89
LYS96	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
R95HA	1.00
R95HB3	1.00
R95HG2	1.00
R95HG3	1.00
R95HD2	1.00
R95HD3	1.00
R95H	1.00
R95HE	1.00
R95HB2	1.00
K96H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG95	HA	1.00	0.136	0.00	0.00
ARG95	HB2	1.00	0.007	1.00	14.73
ARG95	HB3	1.00	0.494	0.00	0.00
ARG95	HG2	1.00	0.026	1.00	12.24
ARG95	HG3	1.00	0.386	0.00	0.00
ARG95	HD2	1.00	0.008	1.00	1.40
ARG95	HD3	1.00	0.008	1.00	1.40
ARG95	H	1.00	0.169	0.00	0.00
LYS96	H	1.00	0.076	0.00	0.00
LYS96	HA	0.66	0.015	1.00	3.96

3.95.8 Detailed Probabilities of ARG95HB3:

Overall probability: 0.222

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG95	0.13	0.89
LYS96	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R95HA	1.00
R95HB2	1.00
R95HG2	1.00
R95HG3	1.00
R95HD2	1.00
R95HD3	1.00
R95H	1.00
R95HE	1.00
R95HB3	1.00
K96H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG95	HA	1.00	0.063	0.00	0.00
ARG95	HB2	1.00	0.066	0.00	0.00
ARG95	HB3	1.00	0.012	1.00	11.43
ARG95	HG2	1.00	0.099	0.00	0.00
ARG95	HG3	1.00	0.459	0.00	0.00
ARG95	HD2	1.00	0.081	0.00	0.00
ARG95	HD3	1.00	0.081	0.00	0.00
ARG95	H	1.00	0.096	0.00	0.00
LYS96	H	1.00	0.003	1.00	-3345797.00

3.95.9 Detailed Probabilities of ARG95HG2:

Overall probability: 0.448

Overall confidence: 0.818

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG95	0.50	0.80
LYS96	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
R95HA	1.00
R95HB2	1.00
R95HB3	1.00
R95HG3	1.00
R95HD2	1.00
R95HD3	1.00
R95H	1.00
R95HE	1.00
R95HH11	1.00
R95HG2	1.00
K96H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG95	HA	1.00	0.157	0.00	0.00
ARG95	HB2	1.00	0.028	1.00	14.73
ARG95	HB3	1.00	0.473	0.00	0.00
ARG95	HG2	1.00	0.005	1.00	12.24
ARG95	HG3	1.00	0.365	0.00	0.00
ARG95	HD2	1.00	0.013	1.00	1.40
ARG95	HD3	1.00	0.013	1.00	1.40
ARG95	H	1.00	0.187	0.00	0.00
LYS96	H	0.97	0.069	0.03	0.00

3.95.10 Detailed Probabilities of ARG95HG3:

Overall probability: 0.750

Overall confidence: 0.800

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG95	0.75	0.80

Expected NOESY Contacts

Proton	Expected probability
R95HA	1.00
R95HB2	1.00
R95HB3	1.00
R95HG2	1.00
R95HD2	1.00
R95HD3	1.00
R95H	1.00
R95HE	1.00
R95HH11	1.00
R95HG3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG95	HA	1.00	0.007	1.00	1.13
ARG95	HB2	1.00	0.013	1.00	1.08
ARG95	HB3	1.00	0.004	1.00	1.04
ARG95	HG2	1.00	0.196	0.00	0.00
ARG95	HG3	1.00	0.164	0.00	0.00
ARG95	HD2	1.00	0.002	1.00	1.17
ARG95	HD3	1.00	0.002	1.00	1.17
ARG95	H	1.00	0.014	1.00	-597132.00

3.95.11 Detailed Probabilities of ARG95HD2:

Overall probability: 0.875

Overall confidence: 0.700

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG95	0.88	0.70

Expected NOESY Contacts

Proton	Expected probability
R95HA	0.98
R95HB2	1.00
R95HB3	1.00
R95HG2	1.00
R95HG3	1.00
R95HD3	1.00
R95HE	1.00
R95HH11	1.00
R95HH21	1.00
R95HD2	1.00

NOESY contacts detailed probability

3.95 ARG(95)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG95	HA	0.97	0.009	1.00	0.25
ARG95	HB2	1.00	0.002	1.00	0.62
ARG95	HB3	1.00	0.001	1.00	0.55
ARG95	HG2	1.00	0.001	1.00	0.89
ARG95	HG3	1.00	0.498	0.00	0.00
ARG95	HD2	1.00	0.002	1.00	28.04
ARG95	HD3	1.00	0.002	1.00	28.04
ARG95	H	0.86	0.004	1.00	-134082.00

3.95.12 Detailed Probabilities of ARG95HD3:

Overall probability: 0.875

Overall confidence: 0.700

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG95	0.88	0.70

Expected NOESY Contacts

Proton	Expected probability
R95HA	0.97
R95HB2	1.00
R95HB3	1.00
R95HG2	1.00
R95HG3	1.00
R95HD2	1.00
R95HE	1.00
R95HH11	1.00
R95HH21	1.00
R95HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG95	HA	0.97	0.009	1.00	0.25
ARG95	HB2	1.00	0.002	1.00	0.62
ARG95	HB3	1.00	0.001	1.00	0.55
ARG95	HG2	1.00	0.001	1.00	0.89
ARG95	HG3	1.00	0.498	0.00	0.00
ARG95	HD2	1.00	0.002	1.00	28.04
ARG95	HD3	1.00	0.002	1.00	28.04
ARG95	H	0.86	0.004	1.00	-134082.00

3.95.13 Detailed Probabilities of ARG95H:

Overall probability: 0.765

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS94	0.86	1.00
ARG95	0.63	1.00
LYS96	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K94HB3	1.00
K94H	1.00
K94HG2	0.96
K94HA	1.00
K94HB2	1.00
R95HA	1.00
R95HB2	1.00
R95HB3	1.00
R95HG2	1.00
R95HG3	1.00
R95H	1.00
K96H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS94	HA	1.00	0.009	1.00	0.17
LYS94	HB2	1.00	0.007	1.00	0.26
LYS94	HB3	1.00	0.007	1.00	0.14
LYS94	HG2	0.96	0.004	1.00	0.10
LYS94	H	1.00	0.043	0.00	0.00
LYS94	HG3	0.94	0.004	1.00	0.10
LYS94	HD2	0.55	0.001	1.00	0.07
ARG95	HA	1.00	0.007	1.00	0.78
ARG95	HB2	1.00	0.007	1.00	0.65
ARG95	HB3	1.00	0.005	1.00	0.68
ARG95	HG2	1.00	0.097	0.00	0.00
ARG95	HG3	1.00	0.407	0.00	0.00
ARG95	H	1.00	0.114	0.00	0.00
ARG95	HD2	0.87	0.005	1.00	0.12
ARG95	HD3	0.86	0.005	1.00	0.12
LYS96	H	1.00	0.010	1.00	-874620.00
LYS96	HB2	0.54	0.001	1.00	0.64



Figure 95: Image from the BMRB

Residue probability: 0.758
Residue probability confidence: 0.943

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	179.034	176.660	3.133	0.000	0.000
CA 3.96.1	58.934	57.014	3.028	0.764	1.000
CB 3.96.2	32.069	32.981	3.186	0.870	1.000
CG 3.96.3	24.910	24.941	1.956	0.900	0.909
CD 3.96.4	28.889	29.020	2.193	0.700	0.889
CE 3.96.5	41.780	41.893	1.492	0.877	0.875
N 3.96.6	119.582	120.954	4.210	0.664	1.000
NZ	NA	—	—	0.000	0.000
HA 3.96.7	4.065	4.262	0.489	0.786	1.000
HB2 3.96.8	1.901	1.774	0.365	0.680	1.000
HB3 3.96.9	1.971	1.742	0.385	0.292	1.000
HG2 3.96.10	1.440	1.358	0.344	0.730	0.909
HG3 3.96.11	1.570	1.343	0.357	0.604	0.909
HD2 3.96.12	1.680	1.614	0.957	0.875	0.889
HD3 3.96.13	1.682	1.595	0.387	0.875	0.889
HE 3.96.14	2.930	2.907	0.230	0.877	0.875
H 3.96.15	7.786	8.185	0.605	0.881	1.000
HZ	NA	—	—	0.000	0.000

3.96.1 Detailed Probabilities of LYS96CA:

Overall probability: 0.764
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG95	0.50	1.00
LYS96	0.89	1.00
ILE97	0.57	1.00

Expected NOESY Contacts

Proton	Expected probability
R95HA	1.00
K96HB2	1.00
K96HB3	1.00
K96HG2	1.00
K96HG3	1.00
K96HD2	0.98
K96HD3	0.98
K96H	1.00
K96HA	1.00
I97HA	1.00
I97H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG95	HA	1.00	0.108	0.00	0.00
ARG95	HB2	0.66	0.015	1.00	3.96
LYS96	HA	1.00	0.023	1.00	41.95
LYS96	HB2	1.00	0.011	1.00	3.96
LYS96	HB3	1.00	0.107	0.00	0.00
LYS96	HG2	1.00	0.001	1.00	1.07
LYS96	HG3	1.00	0.025	1.00	1.73
LYS96	HD2	0.98	0.006	1.00	1.91
LYS96	HD3	0.98	0.004	1.00	1.91
LYS96	H	1.00	0.016	1.00	1.30
LYS96	HE2	0.77	0.007	1.00	0.40
ILE97	HA	1.00	0.104	0.00	0.00
ILE97	H	1.00	0.029	1.00	1.30
ILE97	HG13	0.65	0.033	0.70	0.00

3.96.2 Detailed Probabilities of LYS96CB:

Overall probability: 0.870

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS96	0.86	1.00
ILE97	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K96HA	1.00
K96HB3	1.00
K96HG2	1.00
K96HG3	1.00
K96HD2	1.00
K96HD3	1.00
K96HE2	0.98
K96H	1.00
K96HB2	1.00
I97H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS96	HA	1.00	0.020	1.00	4.53
LYS96	HB2	1.00	0.003	1.00	53.87
LYS96	HB3	1.00	0.067	0.00	0.00
LYS96	HG2	1.00	0.033	0.70	0.00
LYS96	HG3	1.00	0.013	1.00	3.20
LYS96	HD2	1.00	0.003	1.00	5.56
LYS96	HD3	1.00	0.001	1.00	5.56
LYS96	HE2	0.98	0.001	1.00	0.70
LYS96	H	1.00	0.021	1.00	2.95
ILE97	H	1.00	0.024	1.00	2.95

3.96.3 Detailed Probabilities of LYS96CG:

Overall probability: 0.900

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS96	0.89	0.90
ILE97	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K96HA	1.00
K96HB2	1.00
K96HB3	1.00
K96HG3	1.00
K96HD2	1.00
K96HD3	1.00
K96HE2	1.00
K96H	1.00
K96HZ2	1.00
K96HG2	1.00
I97H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS96	HA	1.00	0.023	1.00	0.93
LYS96	HB2	1.00	0.009	1.00	2.94
LYS96	HB3	1.00	0.079	0.00	0.00
LYS96	HG2	1.00	0.029	1.00	52.13
LYS96	HG3	1.00	0.002	1.00	8.71
LYS96	HD2	1.00	0.007	1.00	6.92
LYS96	HD3	1.00	0.005	1.00	6.92
LYS96	HE2	1.00	0.030	1.00	0.86
LYS96	H	1.00	0.023	1.00	0.45
ILE97	H	0.97	0.022	1.00	0.45

3.96.4 Detailed Probabilities of LYS96CD:

Overall probability: 0.700

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS96	0.70	0.89

Expected NOESY Contacts

Proton	Expected probability
K96HA	0.98
K96HB2	1.00
K96HB3	1.00
K96HG2	1.00
K96HG3	1.00
K96HD3	1.00
K96HE2	1.00
K96HZ2	1.00
K96HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS96	HA	0.98	0.017	1.00	1.33
LYS96	HB2	1.00	0.031	0.90	0.00
LYS96	HB3	1.00	0.039	0.10	0.00
LYS96	HG2	1.00	0.037	0.30	0.00
LYS96	HG3	1.00	0.073	0.00	0.00
LYS96	HD2	1.00	0.004	1.00	244.35
LYS96	HD3	1.00	0.002	1.00	244.35
LYS96	HE2	1.00	0.017	1.00	4.26
LYS96	H	0.88	0.023	1.00	0.52

3.96.5 Detailed Probabilities of LYS96CE:

Overall probability: 0.877

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS96	0.88	0.88

Expected NOESY Contacts

Proton	Expected probability
K96HB2	0.98
K96HB3	0.99
K96HG2	1.00
K96HG3	1.00
K96HD2	1.00
K96HD3	1.00
K96HE3	1.00
K96HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS96	HB2	0.99	0.014	1.00	1.28
LYS96	HB3	0.99	0.056	0.01	0.00
LYS96	HG2	1.00	0.029	1.00	1.85
LYS96	HG3	1.00	0.010	1.00	1.96
LYS96	HD2	1.00	0.016	1.00	7.15
LYS96	HD3	1.00	0.018	1.00	7.15
LYS96	HE2	1.00	0.013	1.00	220.78
LYS96	HA	0.76	0.000	1.00	0.98

3.96.6 Detailed Probabilities of LYS96N:

Overall probability: 0.664

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG95	0.41	1.00
LYS96	0.83	1.00
ILE97	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
R95HG2	0.97
R95HA	1.00
R95H	1.00
R95HB3	1.00
R95HB2	1.00
K96HA	1.00
K96HB2	1.00
K96HB3	1.00
K96HG2	1.00
K96HG3	1.00
K96H	1.00
I97H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG95	HA	1.00	0.078	0.00	0.00
ARG95	HB2	1.00	0.076	0.00	0.00
ARG95	HB3	1.00	0.003	1.00	-3345797.00
ARG95	HG2	0.97	0.069	0.03	0.00
ARG95	H	1.00	0.010	1.00	-874620.00
LYS96	HA	1.00	0.007	1.00	-1426214.00
LYS96	HB2	1.00	0.072	0.00	0.00
LYS96	HB3	1.00	0.002	1.00	-3345797.00
LYS96	HG2	1.00	0.007	1.00	-519075.00
LYS96	HG3	1.00	0.003	1.00	-722584.00
LYS96	H	1.00	0.011	1.00	-17394328.00
ILE97	H	1.00	0.034	0.60	0.00
ILE97	HG13	0.59	0.021	1.00	-250370.00

3.96.7 Detailed Probabilities of LYS96HA:

Overall probability: 0.786

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG95	0.67	1.00
LYS96	0.89	1.00
ILE97	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
R95HA	1.00
K96HB2	1.00
K96HB3	1.00
K96HG2	1.00
K96HG3	1.00
K96HD2	0.98
K96HD3	0.98
K96H	1.00
K96HA	1.00
I97HA	1.00
I97H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG95	HA	1.00	0.080	0.00	0.00
ARG95	HB2	0.66	0.023	1.00	0.54
ARG95	HB3	0.81	0.019	1.00	0.47
LYS96	HA	1.00	0.023	1.00	41.95
LYS96	HB2	1.00	0.020	1.00	4.53
LYS96	HB3	1.00	0.461	0.00	0.00
LYS96	HG2	1.00	0.023	1.00	0.93
LYS96	HG3	1.00	0.020	1.00	0.75
LYS96	HD2	0.98	0.017	1.00	1.33
LYS96	HD3	0.98	0.017	1.00	1.33
LYS96	H	1.00	0.007	1.00	-1426214.00
LYS96	HE2	0.77	0.000	1.00	0.98
ILE97	HA	1.00	0.127	0.00	0.00
ILE97	H	1.00	0.007	1.00	-365161.00

3.96.8 Detailed Probabilities of LYS96HB2:

Overall probability: 0.680

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS96	0.76	1.00
ILE97	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K96HA	1.00
K96HB3	1.00
K96HG2	1.00
K96HG3	1.00
K96HD2	1.00
K96HD3	1.00
K96HE2	0.98
K96H	1.00
K96HB2	1.00
I97H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS96	HA	1.00	0.011	1.00	3.96
LYS96	HB2	1.00	0.003	1.00	53.87
LYS96	HB3	1.00	0.897	0.00	0.00
LYS96	HG2	1.00	0.009	1.00	2.94
LYS96	HG3	1.00	0.017	1.00	2.64
LYS96	HD2	1.00	0.031	0.90	0.00
LYS96	HD3	1.00	0.031	0.90	0.00
LYS96	HE2	0.98	0.014	1.00	1.28
LYS96	H	1.00	0.072	0.00	0.00
ILE97	H	1.00	0.066	0.00	0.00

3.96.9 Detailed Probabilities of LYS96HB3:

Overall probability: 0.292

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS96	0.13	1.00
ILE97	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K96HA	1.00
K96HB2	1.00
K96HG2	1.00
K96HG3	1.00
K96HD2	1.00
K96HD3	1.00
K96HE2	0.99
K96H	1.00
K96HB3	1.00
I97H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS96	HA	1.00	0.107	0.00	0.00
LYS96	HB2	1.00	0.067	0.00	0.00
LYS96	HB3	1.00	0.967	0.00	0.00
LYS96	HG2	1.00	0.079	0.00	0.00
LYS96	HG3	1.00	0.053	0.00	0.00
LYS96	HD2	1.00	0.039	0.10	0.00
LYS96	HD3	1.00	0.039	0.10	0.00
LYS96	HE2	0.99	0.056	0.01	0.00
LYS96	H	1.00	0.002	1.00	-3345797.00
ILE97	H	1.00	0.004	1.00	-1741079.00
ILE97	HA	0.85	0.026	1.00	0.07

3.96.10 Detailed Probabilities of LYS96HG2:

Overall probability: 0.730

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS96	0.70	0.90
ILE97	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K96HA	1.00
K96HB2	1.00
K96HB3	1.00
K96HG3	1.00
K96HD2	1.00
K96HD3	1.00
K96HE2	1.00
K96H	1.00
K96HZ2	1.00
K96HG2	1.00
I97H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS96	HA	1.00	0.001	1.00	1.07
LYS96	HB2	1.00	0.033	0.70	0.00
LYS96	HB3	1.00	0.436	0.00	0.00
LYS96	HG2	1.00	0.029	1.00	52.13
LYS96	HG3	1.00	0.019	1.00	7.46
LYS96	HD2	1.00	0.037	0.30	0.00
LYS96	HD3	1.00	0.037	0.30	0.00
LYS96	HE2	1.00	0.029	1.00	1.85
LYS96	H	1.00	0.007	1.00	-519075.00
ILE97	H	0.97	0.029	1.00	-823304.00

3.96.11 Detailed Probabilities of LYS96HG3:

Overall probability: 0.604

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS96	0.67	0.90
ILE97	0.04	1.00

Expected NOESY Contacts

Proton	Expected probability
K96HA	1.00
K96HB2	1.00
K96HB3	1.00
K96HG2	1.00
K96HD2	1.00
K96HD3	1.00
K96HE2	1.00
K96H	1.00
K96HZ2	1.00
K96HG3	1.00
I97H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS96	HA	1.00	0.025	1.00	1.73
LYS96	HB2	1.00	0.013	1.00	3.20
LYS96	HB3	1.00	0.566	0.00	0.00
LYS96	HG2	1.00	0.002	1.00	8.71
LYS96	HG3	1.00	0.010	1.00	37.64
LYS96	HD2	1.00	0.073	0.00	0.00
LYS96	HD3	1.00	0.073	0.00	0.00
LYS96	HE2	1.00	0.010	1.00	1.96
LYS96	H	1.00	0.003	1.00	-722584.00
ILE97	H	0.96	0.101	0.04	0.00

3.96.12 Detailed Probabilities of LYS96HD2:

Overall probability: 0.875

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS96	0.88	0.89

Expected NOESY Contacts

Proton	Expected probability
K96HA	0.98
K96HB2	1.00
K96HB3	1.00
K96HG2	1.00
K96HG3	1.00
K96HD3	1.00
K96HE2	1.00
K96HZ2	1.00
K96HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS96	HA	0.98	0.006	1.00	1.91
LYS96	HB2	1.00	0.003	1.00	5.56
LYS96	HB3	1.00	0.003	1.00	5.56
LYS96	HG2	1.00	0.007	1.00	6.92
LYS96	HG3	1.00	0.055	0.00	0.00
LYS96	HD2	1.00	0.004	1.00	244.35
LYS96	HD3	1.00	0.004	1.00	244.35
LYS96	HE2	1.00	0.016	1.00	7.15

3.96.13 Detailed Probabilities of LYS96HD3:

Overall probability: 0.875

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS96	0.88	0.89

Expected NOESY Contacts

Proton	Expected probability
K96HA	0.98
K96HB2	1.00
K96HB3	1.00
K96HG2	1.00
K96HG3	1.00
K96HD2	1.00
K96HE2	1.00
K96HZ2	1.00
K96HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS96	HA	0.98	0.004	1.00	1.91
LYS96	HB2	1.00	0.001	1.00	5.56
LYS96	HB3	1.00	0.001	1.00	5.56
LYS96	HG2	1.00	0.005	1.00	6.92
LYS96	HG3	1.00	0.057	0.00	0.00
LYS96	HD2	1.00	0.002	1.00	244.35
LYS96	HD3	1.00	0.002	1.00	244.35
LYS96	HE2	1.00	0.018	1.00	7.15

3.96.14 Detailed Probabilities of LYS96HE2:

Overall probability: 0.877

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS96	0.88	0.88

Expected NOESY Contacts

Proton	Expected probability
K96HB2	0.98
K96HB3	0.99
K96HG2	1.00
K96HG3	1.00
K96HD2	1.00
K96HD3	1.00
K96HE3	1.00
K96HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS96	HB2	0.99	0.001	1.00	0.70
LYS96	HB3	0.99	0.674	0.01	0.00
LYS96	HG2	1.00	0.030	1.00	0.86
LYS96	HG3	1.00	0.003	1.00	1.05
LYS96	HD2	1.00	0.017	1.00	4.26
LYS96	HD3	1.00	0.017	1.00	4.26
LYS96	HE2	1.00	0.013	1.00	220.78
LYS96	HA	0.76	0.007	1.00	0.40

3.96.15 Detailed Probabilities of LYS96H:

Overall probability: 0.881

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG95	0.87	1.00
LYS96	1.00	1.00
ILE97	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R95HG2	0.97
R95HA	1.00
R95H	1.00
R95HB3	1.00
R95HB2	1.00
K96HA	1.00
K96HB2	1.00
K96HB3	1.00
K96HG2	1.00
K96HG3	1.00
K96H	1.00
I97H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG95	HA	1.00	0.011	1.00	0.30
ARG95	HB2	1.00	0.004	1.00	0.26
ARG95	HB3	1.00	0.003	1.00	0.33
ARG95	HG2	0.97	0.276	0.03	0.00
ARG95	H	1.00	0.006	1.00	-859333.00
ARG95	HG3	0.95	0.034	0.95	0.00
ARG95	HD2	0.55	0.003	1.00	0.08
ARG95	HD3	0.57	0.003	1.00	0.08
LYS96	HA	1.00	0.016	1.00	1.30
LYS96	HB2	1.00	0.021	1.00	2.95
LYS96	HB3	1.00	0.021	1.00	2.95
LYS96	HG2	1.00	0.023	1.00	0.45
LYS96	HG3	1.00	0.016	1.00	0.50
LYS96	H	1.00	0.011	1.00	-17394328.00
LYS96	HD2	0.88	0.023	1.00	0.52
LYS96	HD3	0.87	0.023	1.00	0.52
ILE97	H	1.00	0.040	0.00	0.00

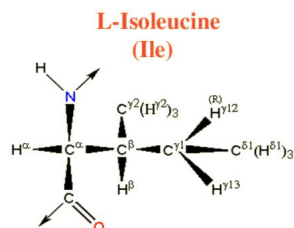


Figure 96: Image from the BMRB

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	178.284	175.926	2.710	0.000	0.000
CA 3.97.1	62.569	61.717	4.152	0.818	1.000
CB 3.97.2	37.206	38.702	3.945	0.922	1.000
CG1 3.97.3	27.265	27.785	2.037	1.000	1.000
CG2 3.97.4	18.753	17.574	1.928	1.000	1.000
CD1 3.97.5	11.899	13.545	3.646	1.000	1.000
N 3.97.6	118.550	121.467	6.098	0.826	1.000
HA 3.97.7	3.938	4.185	1.403	0.900	1.000
HB 3.97.8	1.808	1.776	0.310	1.000	1.000
HG12 3.97.9	1.003	1.271	0.411	0.877	1.000
HG13 3.97.10	0.925	1.186	0.426	0.987	1.000
HG2 3.97.11	0.682	0.762	0.283	0.933	1.000
HD1 3.97.12	0.363	0.668	0.293	1.000	1.000
H 3.97.13	7.831	8.301	0.685	0.975	1.000

3.97.1 Detailed Probabilities of ILE97CA:

Overall probability: 0.818
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS96	0.50	1.00
ILE97	1.00	1.00
GLU98	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K96HA	1.00
I97HB	1.00
I97HG12	1.00
I97HG13	1.00
I97HG21	1.00
I97HD11	0.97
I97H	1.00
I97HA	1.00
E98HA	1.00
E98H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS96	HA	1.00	0.127	0.00	0.00
LYS96	HB3	0.85	0.026	1.00	0.07
ILE97	HA	1.00	0.000	1.00	14.42
ILE97	HB	1.00	0.007	1.00	0.40
ILE97	HG12	1.00	0.003	1.00	0.22
ILE97	HG13	1.00	0.005	1.00	0.43
ILE97	HG21	1.00	0.009	1.00	0.98
ILE97	HD11	0.97	0.005	1.00	0.57
ILE97	H	1.00	0.001	1.00	0.46
GLU98	HA	1.00	0.187	0.00	0.00
GLU98	H	1.00	0.009	1.00	0.21

3.97.2 Detailed Probabilities of ILE97CB:

Overall probability: 0.922

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE97	0.90	1.00
GLU98	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I97HA	1.00
I97HG12	1.00
I97HG13	1.00
I97HG21	1.00
I97HD11	1.00
I97H	1.00
I97HB	1.00
E98H	1.00

NOESY contacts detailed probability

3.97 ILE(97)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE97	HA	1.00	0.005	1.00	0.30
ILE97	HB	1.00	0.011	1.00	5.18
ILE97	HG12	1.00	0.013	1.00	0.36
ILE97	HG13	1.00	0.031	0.90	0.00
ILE97	HG21	1.00	0.036	0.40	0.00
ILE97	HD11	1.00	0.007	1.00	0.41
ILE97	H	1.00	0.000	1.00	0.59
GLU98	H	1.00	0.005	1.00	0.27
GLU98	HA	0.87	0.001	1.00	0.06

3.97.3 Detailed Probabilities of ILE97CG1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE97	1.00	1.00
GLU98	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I97HA	1.00
I97HB	1.00
I97HG13	1.00
I97HG21	1.00
I97HD11	1.00
I97H	1.00
I97HG12	1.00
E98H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE97	HA	1.00	0.014	1.00	0.23
ILE97	HB	1.00	0.018	1.00	0.52
ILE97	HG12	1.00	0.018	1.00	3.42
ILE97	HG13	1.00	0.005	1.00	2.57
ILE97	HG21	1.00	0.005	1.00	0.72
ILE97	HD11	1.00	0.006	1.00	1.03
ILE97	H	1.00	0.001	1.00	0.46
GLU98	H	0.98	0.006	1.00	0.07

3.97.4 Detailed Probabilities of ILE97CG2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE97	1.00	1.00
GLU98	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I97HA	1.00
I97HB	1.00
I97HG12	1.00
I97HG13	1.00
I97HG22	1.00
I97HD11	0.99
I97H	1.00
E98H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE97	HA	1.00	0.008	1.00	0.79
ILE97	HB	1.00	0.007	1.00	1.21
ILE97	HG12	1.00	0.018	1.00	0.38
ILE97	HG13	1.00	0.014	1.00	1.46
ILE97	HG21	1.00	0.002	1.00	25.54
ILE97	HD11	0.99	0.007	1.00	1.84
ILE97	H	1.00	0.002	1.00	0.41
GLU98	H	0.98	0.003	1.00	0.25
GLU98	HA	0.67	0.006	1.00	0.14

3.97.5 Detailed Probabilities of ILE97CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE97	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I97HA	0.97
I97HB	1.00
I97HG12	1.00
I97HG13	1.00
I97HG21	0.99
I97HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE97	HA	0.97	0.008	1.00	0.71
ILE97	HB	1.00	0.003	1.00	0.62
ILE97	HG12	1.00	0.014	1.00	1.02
ILE97	HG13	1.00	0.007	1.00	1.67
ILE97	HG21	0.99	0.003	1.00	1.58
ILE97	HD11	1.00	0.005	1.00	49.53
ILE97	H	0.94	0.003	1.00	0.39

3.97.6 Detailed Probabilities of ILE97N:

Overall probability: 0.826

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS96	0.63	1.00
ILE97	1.00	1.00
GLU98	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K96H	1.00
K96HG2	0.97
K96HG3	0.96
K96HA	1.00
K96HB2	1.00
K96HB3	1.00
I97HA	1.00
I97HB	1.00
I97HG12	1.00
I97HG13	1.00
I97HG21	1.00
I97H	1.00
E98H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS96	HA	1.00	0.007	1.00	-365161.00
LYS96	HB2	1.00	0.066	0.00	0.00
LYS96	HB3	1.00	0.004	1.00	-1741079.00
LYS96	HG2	0.97	0.029	1.00	-823304.00
LYS96	HG3	0.96	0.101	0.04	0.00
LYS96	H	1.00	0.040	0.00	0.00
LYS96	HD2	0.54	0.022	1.00	-1065772.00
LYS96	HD3	0.55	0.020	1.00	-1065772.00
ILE97	HA	1.00	0.001	1.00	-562370.00
ILE97	HB	1.00	0.012	1.00	-772761.00
ILE97	HG12	1.00	0.005	1.00	-423300.00
ILE97	HG13	1.00	0.017	1.00	-738227.00
ILE97	HG21	1.00	0.006	1.00	-336861.00
ILE97	H	1.00	0.005	1.00	-12164598.00
ILE97	HD11	0.94	0.005	1.00	-262683.00
GLU98	H	1.00	0.009	1.00	-561188.00
GLU98	HA	0.93	0.006	1.00	-85119.00

3.97.7 Detailed Probabilities of ILE97HA:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS96	0.00	1.00
ILE97	1.00	1.00
GLU98	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K96HA	1.00
I97HB	1.00
I97HG12	1.00
I97HG13	1.00
I97HG21	1.00
I97HD11	0.97
I97H	1.00
I97HA	1.00
E98HA	1.00
E98H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS96	HA	1.00	0.104	0.00	0.00
ILE97	HA	1.00	0.000	1.00	14.42
ILE97	HB	1.00	0.005	1.00	0.30
ILE97	HG12	1.00	0.014	1.00	0.23
ILE97	HG13	1.00	0.002	1.00	0.21
ILE97	HG21	1.00	0.008	1.00	0.79
ILE97	HD11	0.97	0.008	1.00	0.71
ILE97	H	1.00	0.001	1.00	-562370.00
GLU98	HA	1.00	0.009	1.00	0.06
GLU98	H	1.00	0.010	1.00	-240581.00

3.97.8 Detailed Probabilities of ILE97HB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE97	1.00	1.00
GLU98	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I97HA	1.00
I97HG12	1.00
I97HG13	1.00
I97HG21	1.00
I97HD11	1.00
I97H	1.00
I97HB	1.00
E98H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE97	HA	1.00	0.007	1.00	0.40
ILE97	HB	1.00	0.011	1.00	5.18
ILE97	HG12	1.00	0.018	1.00	0.52
ILE97	HG13	1.00	0.026	1.00	0.90
ILE97	HG21	1.00	0.007	1.00	1.21
ILE97	HD11	1.00	0.003	1.00	0.62
ILE97	H	1.00	0.012	1.00	-772761.00
GLU98	H	1.00	0.007	1.00	-382852.00
GLU98	HA	0.87	0.012	1.00	0.11

3.97.9 Detailed Probabilities of ILE97HG12:

Overall probability: 0.877

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE97	1.00	1.00
GLU98	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
I97HA	1.00
I97HB	1.00
I97HG13	1.00
I97HG21	1.00
I97HD11	1.00
I97H	1.00
I97HG12	1.00
E98H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE97	HA	1.00	0.003	1.00	0.22
ILE97	HB	1.00	0.013	1.00	0.36
ILE97	HG12	1.00	0.018	1.00	3.42
ILE97	HG13	1.00	0.014	1.00	2.24
ILE97	HG21	1.00	0.018	1.00	0.38
ILE97	HD11	1.00	0.014	1.00	1.02
ILE97	H	1.00	0.005	1.00	-423300.00
GLU98	H	0.98	0.083	0.02	0.00

3.97.10 Detailed Probabilities of ILE97HG13:

Overall probability: 0.987

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE97	0.99	1.00
GLU98	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I97HA	1.00
I97HB	1.00
I97HG12	1.00
I97HG21	1.00
I97HD11	1.00
I97H	1.00
I97HG13	1.00
E98H	0.95

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE97	HA	1.00	0.005	1.00	0.43
ILE97	HB	1.00	0.031	0.90	0.00
ILE97	HG12	1.00	0.005	1.00	2.57
ILE97	HG13	1.00	0.005	1.00	5.21
ILE97	HG21	1.00	0.014	1.00	1.46
ILE97	HD11	1.00	0.007	1.00	1.67
ILE97	H	1.00	0.017	1.00	-738227.00
GLU98	H	0.95	0.005	1.00	-307212.00

3.97.11 Detailed Probabilities of ILE97HG21:

Overall probability: 0.933

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE97	0.91	1.00
GLU98	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I97HA	1.00
I97HB	1.00
I97HG12	1.00
I97HG13	1.00
I97HG22	1.00
I97HD11	0.99
I97H	1.00
E98H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE97	HA	1.00	0.009	1.00	0.98
ILE97	HB	1.00	0.036	0.40	0.00
ILE97	HG12	1.00	0.005	1.00	0.72
ILE97	HG13	1.00	0.024	1.00	0.91
ILE97	HG21	1.00	0.002	1.00	25.54
ILE97	HD11	0.99	0.003	1.00	1.58
ILE97	H	1.00	0.006	1.00	-336861.00
GLU98	H	0.98	0.005	1.00	-231628.00
GLU98	HA	0.67	0.003	1.00	0.18

3.97.12 Detailed Probabilities of ILE97HD11:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE97	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I97HA	0.97
I97HB	1.00
I97HG12	1.00
I97HG13	1.00
I97HG21	0.99
I97HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE97	HA	0.97	0.005	1.00	0.57
ILE97	HB	1.00	0.007	1.00	0.41
ILE97	HG12	1.00	0.006	1.00	1.03
ILE97	HG13	1.00	0.007	1.00	0.89
ILE97	HG21	0.99	0.007	1.00	1.84
ILE97	HD11	1.00	0.005	1.00	49.53
ILE97	H	0.94	0.005	1.00	-262683.00

3.97.13 Detailed Probabilities of ILE97H:

Overall probability: 0.975

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS96	0.95	1.00
ILE97	1.00	1.00
GLU98	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K96H	1.00
K96HG2	0.97
K96HG3	0.96
K96HA	1.00
K96HB2	1.00
K96HB3	1.00
I97HA	1.00
I97HB	1.00
I97HG12	1.00
I97HG13	1.00
I97HG21	1.00
I97H	1.00
E98H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS96	HA	1.00	0.029	1.00	1.30
LYS96	HB2	1.00	0.024	1.00	2.95
LYS96	HB3	1.00	0.024	1.00	2.95
LYS96	HG2	0.97	0.022	1.00	0.45
LYS96	HG3	0.96	0.029	1.00	0.50
LYS96	H	1.00	0.034	0.60	0.00
LYS96	HD2	0.54	0.022	1.00	0.52
LYS96	HD3	0.55	0.022	1.00	0.52
ILE97	HA	1.00	0.001	1.00	0.46
ILE97	HB	1.00	0.000	1.00	0.59
ILE97	HG12	1.00	0.001	1.00	0.46
ILE97	HG13	1.00	0.001	1.00	0.44
ILE97	HG21	1.00	0.002	1.00	0.41
ILE97	H	1.00	0.005	1.00	-12164598.00
ILE97	HD11	0.94	0.003	1.00	0.39
GLU98	H	1.00	0.003	1.00	-669036.00

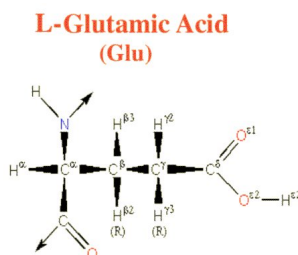


Figure 97: Image from the BMRB

Residue probability: 0.798
Residue probability confidence: 0.925

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	180.040	176.942	2.547	0.000	0.000
CA 3.98.1	58.950	57.442	3.837	0.818	1.000
CB 3.98.2	29.435	30.185	4.018	0.875	0.875
CG 3.98.3	36.433	36.085	1.533	0.714	0.875
N 3.98.4	121.984	120.574	4.837	0.858	1.000
HA 3.98.5	4.336	4.245	0.429	0.833	1.000
HB2 3.98.6	2.179	2.021	0.233	1.000	0.875
HB3 3.98.7	2.053	1.994	0.244	0.814	0.875
HG2 3.98.8	2.377	2.258	0.226	0.571	0.875
HG3 3.98.9	2.437	2.233	0.232	0.571	0.875
H 3.98.10	8.670	8.332	0.601	0.927	1.000
HE2	NA	—	—	0.000	0.000

3.98.1 Detailed Probabilities of GLU98CA:

Overall probability: 0.818
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE97	1.00	1.00
GLU98	0.83	1.00
SER99	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
I97HA	1.00
E98HB2	1.00
E98HB3	1.00
E98HG2	1.00
E98HG3	1.00
E98H	1.00
E98HA	1.00
S99HA	1.00
S99H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE97	HA	1.00	0.009	1.00	0.06
ILE97	HB	0.87	0.012	1.00	0.11
ILE97	HG21	0.69	0.003	1.00	0.18
GLU98	HA	1.00	0.001	1.00	10.15
GLU98	HB2	1.00	0.009	1.00	0.80
GLU98	HB3	1.00	0.008	1.00	1.10
GLU98	HG2	1.00	0.004	1.00	0.89
GLU98	HG3	1.00	0.064	0.00	0.00
GLU98	H	1.00	0.005	1.00	0.59
SER99	HA	1.00	0.006	1.00	10.15
SER99	H	1.00	0.160	0.00	0.00

3.98.2 Detailed Probabilities of GLU98CB:

Overall probability: 0.875

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU98	1.00	0.86
SER99	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E98HA	1.00
E98HB3	1.00
E98HG2	1.00
E98HG3	1.00
E98H	1.00
E98HE2	1.00
E98HB2	1.00
S99H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU98	HA	1.00	0.003	1.00	1.86
GLU98	HB2	1.00	0.003	1.00	19.33
GLU98	HB3	1.00	0.003	1.00	12.14
GLU98	HG2	1.00	0.027	1.00	1.77
GLU98	HG3	1.00	0.024	1.00	2.85
GLU98	H	1.00	0.002	1.00	0.79
SER99	H	1.00	0.067	0.00	0.00
SER99	HA	0.70	0.004	1.00	1.86

3.98.3 Detailed Probabilities of GLU98CG:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU98	0.67	0.86
SER99	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E98HA	1.00
E98HB2	1.00
E98HB3	1.00
E98HG3	1.00
E98H	1.00
E98HE2	1.00
E98HG2	1.00
S99H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU98	HA	1.00	0.003	1.00	0.94
GLU98	HB2	1.00	0.010	1.00	5.21
GLU98	HB3	1.00	0.108	0.00	0.00
GLU98	HG2	1.00	0.014	1.00	30.23
GLU98	HG3	1.00	0.046	0.00	0.00
GLU98	H	1.00	0.003	1.00	0.36
SER99	H	0.97	0.020	1.00	0.13

3.98.4 Detailed Probabilities of GLU98N:

Overall probability: 0.858

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE97	0.84	1.00
GLU98	0.83	1.00
SER99	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I97HG13	0.95
I97HG22	0.98
I97HA	1.00
I97HG12	0.98
I97HB	1.00
I97H	1.00
E98HA	1.00
E98HB2	1.00
E98HB3	1.00
E98HG2	1.00
E98HG3	1.00
E98H	1.00
S99H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE97	HA	1.00	0.010	1.00	-240581.00
ILE97	HB	1.00	0.007	1.00	-382852.00
ILE97	HG12	0.98	0.083	0.02	0.00
ILE97	HG13	0.95	0.005	1.00	-307212.00
ILE97	HG21	0.99	0.005	1.00	-231628.00
ILE97	H	1.00	0.003	1.00	-669036.00
GLU98	HA	1.00	0.000	1.00	-594495.00
GLU98	HB2	1.00	0.002	1.00	-724848.00
GLU98	HB3	1.00	0.006	1.00	-518208.00
GLU98	HG2	1.00	0.048	0.00	0.00
GLU98	HG3	1.00	0.012	1.00	-425953.00
GLU98	H	1.00	0.003	1.00	-4573971.00
SER99	H	1.00	0.009	1.00	-355639.00
SER99	HA	0.86	0.007	1.00	-594495.00

3.98.5 Detailed Probabilities of GLU98HA:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE97	0.75	1.00
GLU98	1.00	1.00
SER99	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
I97HA	1.00
E98HB2	1.00
E98HB3	1.00
E98HG2	1.00
E98HG3	1.00
E98H	1.00
E98HA	1.00
S99HA	1.00
S99H	1.00

NOESY contacts detailed probability

3.98 GLU(98)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE97	HA	1.00	0.187	0.00	0.00
ILE97	HB	0.87	0.001	1.00	0.06
ILE97	HG21	0.69	0.006	1.00	0.14
ILE97	H	0.93	0.006	1.00	-85119.00
GLU98	HA	1.00	0.001	1.00	10.15
GLU98	HB2	1.00	0.003	1.00	1.86
GLU98	HB3	1.00	0.002	1.00	2.30
GLU98	HG2	1.00	0.003	1.00	0.94
GLU98	HG3	1.00	0.003	1.00	0.42
GLU98	H	1.00	0.000	1.00	-594495.00
SER99	HA	1.00	0.158	0.00	0.00
SER99	H	1.00	0.004	1.00	-1133548.00

3.98.6 Detailed Probabilities of GLU98HB2:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU98	1.00	0.86
SER99	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E98HA	1.00
E98HB3	1.00
E98HG2	1.00
E98HG3	1.00
E98H	1.00
E98HE2	1.00
E98HB2	1.00
S99H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU98	HA	1.00	0.009	1.00	0.80
GLU98	HB2	1.00	0.003	1.00	19.33
GLU98	HB3	1.00	0.003	1.00	14.03
GLU98	HG2	1.00	0.010	1.00	5.21
GLU98	HG3	1.00	0.001	1.00	2.93
GLU98	H	1.00	0.002	1.00	-724848.00
SER99	H	1.00	0.003	1.00	-383878.00

3.98.7 Detailed Probabilities of GLU98HB3:

Overall probability: 0.814

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU98	0.78	0.86
SER99	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E98HA	1.00
E98HB2	1.00
E98HG2	1.00
E98HG3	1.00
E98H	1.00
E98HE2	1.00
E98HB3	1.00
S99H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU98	HA	1.00	0.008	1.00	1.10
GLU98	HB2	1.00	0.003	1.00	12.14
GLU98	HB3	1.00	0.012	1.00	52.03
GLU98	HG2	1.00	0.108	0.00	0.00
GLU98	HG3	1.00	0.033	0.70	0.00
GLU98	H	1.00	0.006	1.00	-518208.00
SER99	H	1.00	0.007	1.00	-359132.00

3.98.8 Detailed Probabilities of GLU98HG2:

Overall probability: 0.571

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU98	0.50	0.86
SER99	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E98HA	1.00
E98HB2	1.00
E98HB3	1.00
E98HG3	1.00
E98H	1.00
E98HE2	1.00
E98HG2	1.00
S99H	0.97

NOESY contacts detailed probability

3.98 GLU(98)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU98	HA	1.00	0.004	1.00	0.89
GLU98	HB2	1.00	0.027	1.00	1.77
GLU98	HB3	1.00	0.042	0.00	0.00
GLU98	HG2	1.00	0.014	1.00	30.23
GLU98	HG3	1.00	0.068	0.00	0.00
GLU98	H	1.00	0.048	0.00	0.00
SER99	H	0.97	0.003	1.00	-174682.00

3.98.9 Detailed Probabilities of GLU98HG3:

Overall probability: 0.571

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU98	0.50	0.86
SER99	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E98HA	1.00
E98HB2	1.00
E98HB3	1.00
E98HG2	1.00
E98H	1.00
E98HE2	1.00
E98HG3	1.00
S99H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU98	HA	1.00	0.064	0.00	0.00
GLU98	HB2	1.00	0.024	1.00	2.85
GLU98	HB3	1.00	0.102	0.00	0.00
GLU98	HG2	1.00	0.046	0.00	0.00
GLU98	HG3	1.00	0.008	1.00	35.10
GLU98	H	1.00	0.012	1.00	-425953.00
SER99	H	0.97	0.000	1.00	-154382.00

3.98.10 Detailed Probabilities of GLU98H:

Overall probability: 0.927

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE97	0.84	1.00
GLU98	1.00	1.00
SER99	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I97HG13	0.95
I97HG22	0.98
I97HA	1.00
I97HG12	0.98
I97HB	1.00
I97H	1.00
E98HA	1.00
E98HB2	1.00
E98HB3	1.00
E98HG2	1.00
E98HG3	1.00
E98H	1.00
S99H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE97	HA	1.00	0.009	1.00	0.21
ILE97	HB	1.00	0.005	1.00	0.27
ILE97	HG12	0.98	0.006	1.00	0.07
ILE97	HG13	0.95	0.137	0.05	0.00
ILE97	HG21	0.99	0.003	1.00	0.25
ILE97	H	1.00	0.009	1.00	-561188.00
GLU98	HA	1.00	0.005	1.00	0.59
GLU98	HB2	1.00	0.002	1.00	0.79
GLU98	HB3	1.00	0.030	1.00	1.18
GLU98	HG2	1.00	0.003	1.00	0.36
GLU98	HG3	1.00	0.008	1.00	0.26
GLU98	H	1.00	0.003	1.00	-4573971.00
SER99	H	1.00	0.006	1.00	-502796.00

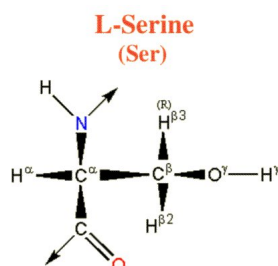
3.99 SER(99)

Figure 98: Image from the BMRB

Residue probability: 0.686

Residue probability confidence: 0.855

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.820	174.682	1.868	0.000	0.000
CA 3.99.1	60.410	58.750	3.025	0.333	0.857
CB 3.99.2	62.680	63.523	4.288	0.580	0.800
N 3.99.3	115.499	116.135	5.326	1.000	0.909
HA 3.99.4	4.343	4.486	0.430	0.856	0.857
HB 3.99.5	3.996	3.856	0.325	0.600	0.800
H 3.99.6	8.099	8.292	0.600	0.745	0.909
HG	NA	—	—	0.000	0.000

3.99.1 Detailed Probabilities of SER99CA:

Overall probability: 0.333

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU98	0.00	1.00
SER99	0.67	0.75
GLN100	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E98HA	1.00
S99HB2	1.00
S99H	1.00
S99HG	1.00
S99HA	1.00
Q100HA	1.00
Q100H	1.00

NOESY contacts detailed probability

3.99 SER(99)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU98	HA	1.00	0.158	0.00	0.00
SER99	HA	1.00	0.151	0.00	0.00
SER99	HB2	1.00	0.015	1.00	2.23
SER99	H	1.00	0.010	1.00	1.34
GLN100	HA	1.00	0.184	0.00	0.00
GLN100	H	1.00	0.177	0.00	0.00

3.99.2 Detailed Probabilities of SER99CB:

Overall probability: 0.580

Overall confidence: 0.800

Inter- and intra-residue probability

Residue	Probability	Confidence
SER99	0.67	0.75
GLN100	0.45	1.00

Expected NOESY Contacts

Proton	Expected probability
S99HA	1.00
S99HB3	1.00
S99H	1.00
S99HG	1.00
Q100H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER99	HA	1.00	0.002	1.00	1.64
SER99	HB2	1.00	0.257	0.00	0.00
SER99	H	1.00	0.007	1.00	0.61
GLN100	H	1.00	0.483	0.00	0.00
GLN100	HA	0.74	0.031	0.90	0.00

3.99.3 Detailed Probabilities of SER99N:

Overall probability: 1.000

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU98	1.00	1.00
SER99	1.00	0.75
GLN100	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E98HB2	1.00
E98HG3	0.97
E98HA	1.00
E98H	1.00
E98HG2	0.97
E98HB3	1.00
S99HA	1.00
S99HB2	1.00
S99HG	1.00
S99H	1.00
Q100H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU98	HA	1.00	0.004	1.00	-1133548.00
GLU98	HB2	1.00	0.003	1.00	-383878.00
GLU98	HB3	1.00	0.007	1.00	-359132.00
GLU98	HG2	0.97	0.003	1.00	-174682.00
GLU98	HG3	0.97	0.000	1.00	-154382.00
GLU98	H	1.00	0.006	1.00	-502796.00
SER99	HA	1.00	0.003	1.00	-1133548.00
SER99	HB2	1.00	0.008	1.00	-890001.00
SER99	H	1.00	0.008	1.00	-5567625.00
GLN100	H	1.00	0.003	1.00	-354496.00
GLN100	HB2	0.57	0.028	1.00	-383878.00

3.99.4 Detailed Probabilities of SER99HA:

Overall probability: 0.856

Overall confidence: 0.857

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU98	1.00	1.00
SER99	0.67	0.75
GLN100	0.85	1.00

Expected NOESY Contacts

Proton	Expected probability
E98HA	1.00
S99HB2	1.00
S99H	1.00
S99HG	1.00
S99HA	1.00
Q100HA	1.00
Q100H	1.00

NOESY contacts detailed probability

3.99 SER(99)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU98	HA	1.00	0.006	1.00	10.15
GLU98	HB2	0.70	0.004	1.00	1.86
GLU98	HB3	0.82	0.005	1.00	2.30
GLU98	H	0.86	0.007	1.00	-594495.00
SER99	HA	1.00	0.151	0.00	0.00
SER99	HB2	1.00	0.002	1.00	1.64
SER99	H	1.00	0.003	1.00	-1133548.00
GLN100	HA	1.00	0.033	0.70	0.00
GLN100	H	1.00	0.018	1.00	-314006.00

3.99.5 Detailed Probabilities of SER99HB2:

Overall probability: 0.600

Overall confidence: 0.800

Inter- and intra-residue probability

Residue	Probability	Confidence
SER99	0.67	0.75
GLN100	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
S99HA	1.00
S99HB3	1.00
S99H	1.00
S99HG	1.00
Q100H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER99	HA	1.00	0.015	1.00	2.23
SER99	HB2	1.00	0.257	0.00	0.00
SER99	H	1.00	0.008	1.00	-890001.00
GLN100	H	1.00	0.198	0.00	0.00
GLN100	HA	0.74	0.011	1.00	0.06

3.99.6 Detailed Probabilities of SER99H:

Overall probability: 0.745

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU98	0.53	1.00
SER99	1.00	0.75
GLN100	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E98HB2	1.00
E98HG3	0.97
E98HA	1.00
E98H	1.00
E98HG2	0.97
E98HB3	1.00
S99HA	1.00
S99HB2	1.00
S99HG	1.00
S99H	1.00
Q100H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU98	HA	1.00	0.160	0.00	0.00
GLU98	HB2	1.00	0.067	0.00	0.00
GLU98	HB3	1.00	0.003	1.00	1.37
GLU98	HG2	0.97	0.020	1.00	0.13
GLU98	HG3	0.97	0.038	0.20	0.00
GLU98	H	1.00	0.009	1.00	-355639.00
SER99	HA	1.00	0.010	1.00	1.34
SER99	HB2	1.00	0.007	1.00	0.61
SER99	H	1.00	0.008	1.00	-5567625.00
GLN100	H	1.00	0.016	1.00	-336011.00
GLN100	HA	0.82	0.012	1.00	0.42

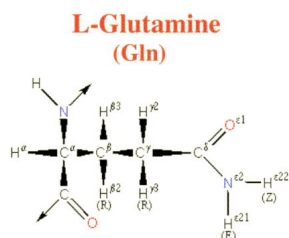


Figure 99: Image from the BMRB

Residue probability: 0.706
Residue probability confidence: 0.986

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	175.857	176.405	1.998	0.000	0.000
CA 3.100.1	55.926	56.667	2.318	0.669	1.000
CB 3.100.2	29.212	29.436	2.799	0.800	1.000
CG 3.100.3	34.179	33.781	1.871	0.875	1.000
N 3.100.4	119.301	119.799	3.762	0.627	0.909
NE2 3.100.5	110.232	111.924	2.434	0.857	1.000
HA 3.100.6	4.310	4.265	0.455	0.915	1.000
HB2 3.100.7	2.210	2.047	0.290	0.667	1.000
HB3 3.100.8	2.048	2.012	0.313	0.556	1.000
HG2 3.100.9	2.441	2.308	0.289	0.625	1.000
HG3 3.100.10	2.351	2.284	0.313	0.625	1.000
H 3.100.11	7.623	8.232	0.711	0.660	0.909
HE21 3.100.12	7.286	7.217	0.496	0.714	1.000
HE22 3.100.13	6.755	7.041	0.463	0.583	1.000

3.100.1 Detailed Probabilities of GLN100CA:

Overall probability: 0.669
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
SER99	0.90	1.00
GLN100	0.43	1.00
GLY101	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S99HA	1.00
Q100HB2	1.00
Q100HB3	1.00
Q100HG2	1.00
Q100HG3	1.00
Q100H	1.00
Q100HA	1.00
G101H	1.00
G101HA2	1.00
G101HA3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER99	HA	1.00	0.033	0.70	0.00
SER99	HB2	0.63	0.011	1.00	0.06
SER99	H	0.82	0.012	1.00	0.42
GLN100	HA	1.00	0.000	1.00	21.81
GLN100	HB2	1.00	0.859	0.00	0.00
GLN100	HB3	1.00	1.021	0.00	0.00
GLN100	HG2	1.00	0.628	0.00	0.00
GLN100	HG3	1.00	0.718	0.00	0.00
GLN100	H	1.00	0.002	1.00	0.34
GLN100	HE21	0.94	0.007	1.00	0.07
GLY101	HA2	1.00	0.005	1.00	0.06
GLY101	HA3	1.00	0.002	1.00	0.06
GLY101	H	1.00	0.001	1.00	0.29

3.100.2 Detailed Probabilities of GLN100CB:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN100	0.78	1.00
GLY101	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q100HA	1.00
Q100HB3	1.00
Q100HG2	1.00
Q100HG3	1.00
Q100H	1.00
Q100HE21	1.00
Q100HE22	1.00
Q100HB2	1.00
G101H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN100	HA	1.00	0.029	1.00	1.86
GLN100	HB2	1.00	0.028	1.00	19.33
GLN100	HB3	1.00	0.008	1.00	12.14
GLN100	HG2	1.00	0.028	1.00	2.85
GLN100	HG3	1.00	0.001	1.00	1.77
GLN100	H	1.00	0.009	1.00	0.92
GLN100	HE21	1.00	0.302	0.00	0.00
GLN100	HE22	1.00	0.038	0.20	0.00
GLY101	H	1.00	0.004	1.00	0.09

3.100.3 Detailed Probabilities of GLN100CG:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN100	0.88	1.00

Expected NOESY Contacts

Proton	Expected probability
Q100HA	1.00
Q100HB2	1.00
Q100HB3	1.00
Q100HG3	1.00
Q100H	1.00
Q100HE21	1.00
Q100HE22	1.00
Q100HG2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN100	HA	1.00	0.005	1.00	0.60
GLN100	HB2	1.00	0.020	1.00	4.31
GLN100	HB3	1.00	0.008	1.00	2.35
GLN100	HG2	1.00	0.025	1.00	103.18
GLN100	HG3	1.00	0.065	0.00	0.00
GLN100	H	1.00	0.010	1.00	0.76
GLN100	HE21	1.00	0.005	1.00	0.17
GLN100	HE22	1.00	0.006	1.00	0.11

3.100.4 Detailed Probabilities of GLN100N:

Overall probability: 0.627

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
SER99	0.67	0.75
GLN100	0.65	1.00
GLY101	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
S99HA	1.00
S99HB2	1.00
S99HG	0.96
S99H	1.00
Q100HA	1.00
Q100HB2	1.00
Q100HB3	1.00
Q100HG2	1.00
Q100HG3	1.00
Q100H	1.00
G101H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER99	HA	1.00	0.018	1.00	-314006.00
SER99	HB2	1.00	0.198	0.00	0.00
SER99	H	1.00	0.016	1.00	-336011.00
GLN100	HA	1.00	0.015	1.00	-314006.00
GLN100	HB2	1.00	0.139	0.00	0.00
GLN100	HB3	1.00	0.007	1.00	-400677.00
GLN100	HG2	1.00	0.092	0.00	0.00
GLN100	HG3	1.00	0.002	1.00	-176011.00
GLN100	H	1.00	0.031	0.90	0.00
GLY101	H	1.00	0.061	0.00	0.00
GLY101	HA2	0.73	0.010	1.00	-298211.00

3.100.5 Detailed Probabilities of GLN100NE2:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN100	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
Q100HB2	1.00
Q100HB3	1.00
Q100HG2	1.00
Q100HG3	1.00
Q100HE22	1.00
Q100HE21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN100	HB2	1.00	0.014	1.00	-87167.00
GLN100	HB3	1.00	0.176	0.00	0.00
GLN100	HG2	1.00	0.003	1.00	-226629.00
GLN100	HG3	1.00	0.001	1.00	-204096.00
GLN100	HE21	1.00	0.003	1.00	-17246640.00
GLN100	HE22	1.00	0.003	1.00	-10993139.00
GLN100	HA	0.94	0.014	1.00	-83677.00

3.100.6 Detailed Probabilities of GLN100HA:

Overall probability: 0.915

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
SER99	0.63	1.00
GLN100	1.00	1.00
GLY101	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S99HA	1.00
Q100HB2	1.00
Q100HB3	1.00
Q100HG2	1.00
Q100HG3	1.00
Q100H	1.00
Q100HA	1.00
G101H	1.00
G101HA2	1.00
G101HA3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER99	HA	1.00	0.184	0.00	0.00
SER99	HB2	0.63	0.031	0.90	0.00
SER99	H	0.82	0.030	1.00	0.00
GLN100	HA	1.00	0.000	1.00	21.81
GLN100	HB2	1.00	0.029	1.00	1.86
GLN100	HB3	1.00	0.023	1.00	0.59
GLN100	HG2	1.00	0.005	1.00	0.60
GLN100	HG3	1.00	0.001	1.00	0.65
GLN100	H	1.00	0.015	1.00	-314006.00
GLN100	HE21	0.94	0.014	1.00	-83677.00
GLY101	HA2	1.00	0.002	1.00	0.15
GLY101	HA3	1.00	0.024	1.00	0.09
GLY101	H	1.00	0.014	1.00	-719690.00

3.100.7 Detailed Probabilities of GLN100HB2:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN100	0.63	1.00
GLY101	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q100HA	1.00
Q100HB3	1.00
Q100HG2	1.00
Q100HG3	1.00
Q100H	1.00
Q100HE21	1.00
Q100HE22	1.00
Q100HB2	1.00
G101H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN100	HA	1.00	0.859	0.00	0.00
GLN100	HB2	1.00	0.028	1.00	19.33
GLN100	HB3	1.00	0.028	1.00	14.03
GLN100	HG2	1.00	0.020	1.00	4.31
GLN100	HG3	1.00	0.030	1.00	0.00
GLN100	H	1.00	0.139	0.00	0.00
GLN100	HE21	1.00	0.014	1.00	-87167.00
GLN100	HE22	1.00	0.137	0.00	0.00
GLY101	H	1.00	0.009	1.00	-78768.00

3.100.8 Detailed Probabilities of GLN100HB3:

Overall probability: 0.556

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN100	0.50	1.00
GLY101	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q100HA	1.00
Q100HB2	1.00
Q100HG2	1.00
Q100HG3	1.00
Q100H	1.00
Q100HE21	1.00
Q100HE22	1.00
Q100HB3	1.00
G101H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN100	HA	1.00	1.021	0.00	0.00
GLN100	HB2	1.00	0.008	1.00	12.14
GLN100	HB3	1.00	0.007	1.00	52.03
GLN100	HG2	1.00	0.008	1.00	2.35
GLN100	HG3	1.00	0.192	0.00	0.00
GLN100	H	1.00	0.007	1.00	-400677.00
GLN100	HE21	1.00	0.176	0.00	0.00
GLN100	HE22	1.00	0.299	0.00	0.00
GLY101	H	1.00	0.005	1.00	-116122.00

3.100.9 Detailed Probabilities of GLN100HG2:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN100	0.63	1.00

Expected NOESY Contacts

Proton	Expected probability
Q100HA	1.00
Q100HB2	1.00
Q100HB3	1.00
Q100HG3	1.00
Q100H	1.00
Q100HE21	1.00
Q100HE22	1.00
Q100HG2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN100	HA	1.00	0.628	0.00	0.00
GLN100	HB2	1.00	0.028	1.00	2.85
GLN100	HB3	1.00	0.106	0.00	0.00
GLN100	HG2	1.00	0.025	1.00	103.18
GLN100	HG3	1.00	0.001	1.00	4.45
GLN100	H	1.00	0.092	0.00	0.00
GLN100	HE21	1.00	0.003	1.00	-226629.00
GLN100	HE22	1.00	0.004	1.00	-185646.00

3.100.10 Detailed Probabilities of GLN100HG3:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN100	0.63	1.00

Expected NOESY Contacts

Proton	Expected probability
Q100HA	1.00
Q100HB2	1.00
Q100HB3	1.00
Q100HG2	1.00
Q100H	1.00
Q100HE21	1.00
Q100HE22	1.00
Q100HG3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN100	HA	1.00	0.718	0.00	0.00
GLN100	HB2	1.00	0.001	1.00	1.77
GLN100	HB3	1.00	0.016	1.00	4.32
GLN100	HG2	1.00	0.065	0.00	0.00
GLN100	HG3	1.00	0.089	0.00	0.00
GLN100	H	1.00	0.002	1.00	-176011.00
GLN100	HE21	1.00	0.001	1.00	-204096.00
GLN100	HE22	1.00	0.004	1.00	-167488.00

3.100.11 Detailed Probabilities of GLN100H:

Overall probability: 0.660

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
SER99	0.33	0.75
GLN100	0.77	1.00
GLY101	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S99HA	1.00
S99HB2	1.00
S99HG	0.96
S99H	1.00
Q100HA	1.00
Q100HB2	1.00
Q100HB3	1.00
Q100HG2	1.00
Q100HG3	1.00
Q100H	1.00
G101H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER99	HA	1.00	0.177	0.00	0.00
SER99	HB2	1.00	0.483	0.00	0.00
SER99	H	1.00	0.003	1.00	-354496.00
GLN100	HA	1.00	0.002	1.00	0.34
GLN100	HB2	1.00	0.009	1.00	0.92
GLN100	HB3	1.00	0.033	0.70	0.00
GLN100	HG2	1.00	0.010	1.00	0.76
GLN100	HG3	1.00	0.334	0.00	0.00
GLN100	H	1.00	0.031	0.90	0.00
GLY101	H	1.00	0.010	1.00	-1129537.00

3.100.12 Detailed Probabilities of GLN100HE21:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN100	0.71	1.00

Expected NOESY Contacts

Proton	Expected probability
Q100HB2	1.00
Q100HB3	1.00
Q100HG2	1.00
Q100HG3	1.00
Q100HE22	1.00
Q100HE21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN100	HB2	1.00	0.302	0.00	0.00
GLN100	HB3	1.00	0.098	0.00	0.00
GLN100	HG2	1.00	0.005	1.00	0.17
GLN100	HG3	1.00	0.003	1.00	0.16
GLN100	HE21	1.00	0.003	1.00	-17246640.00
GLN100	HE22	1.00	0.002	1.00	-12661910.00
GLN100	HA	0.94	0.007	1.00	0.07

3.100.13 Detailed Probabilities of GLN100HE22:**Overall probability:** 0.583**Overall confidence:** 1.000**Inter- and intra-residue probability**

Residue	Probability	Confidence
GLN100	0.58	1.00

Expected NOESY Contacts

Proton	Expected probability
Q100HB2	1.00
Q100HB3	1.00
Q100HG2	1.00
Q100HG3	1.00
Q100HE21	1.00
Q100HE22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN100	HB2	1.00	0.038	0.20	0.00
GLN100	HB3	1.00	0.037	0.30	0.00
GLN100	HG2	1.00	0.006	1.00	0.11
GLN100	HG3	1.00	0.000	1.00	0.14
GLN100	HE21	1.00	0.003	1.00	-10993139.00
GLN100	HE22	1.00	0.130	0.00	0.00

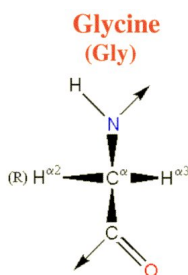


Figure 100: Image from the BMRB

Residue probability: 0.900
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	173.748	173.872	2.493	0.000	0.000
CA 3.101.1	45.203	45.581	4.381	1.000	1.000
N 3.101.2	105.765	109.752	5.331	1.000	1.000
HA2 3.101.3	3.722	3.967	0.380	0.875	1.000
HA3 3.101.4	4.009	3.897	0.390	1.000	1.000
H 3.101.5	7.945	8.343	0.939	0.625	1.000

3.101.1 Detailed Probabilities of GLY101CA:

Overall probability: 1.000
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN100	1.00	1.00
GLY101	1.00	1.00
TYR102	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q100HA	1.00
G101HA3	1.00
G101H	1.00
G101HA2	1.00
Y102HA	1.00
Y102H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN100	HA	1.00	0.002	1.00	0.15
GLY101	HA2	1.00	0.006	1.00	2.39
GLY101	HA3	1.00	0.001	1.00	2.28
GLY101	H	1.00	0.001	1.00	0.57
TYR102	HA	1.00	0.002	1.00	0.10
TYR102	H	1.00	0.009	1.00	0.14

3.101.2 Detailed Probabilities of GLY101N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN100	1.00	1.00
GLY101	1.00	1.00
TYR102	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q100HB3	1.00
Q100H	1.00
Q100HA	1.00
Q100HB2	1.00
G101HA2	1.00
G101HA3	1.00
G101H	1.00
Y102H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN100	HA	1.00	0.014	1.00	-719690.00
GLN100	HB2	1.00	0.009	1.00	-78768.00
GLN100	HB3	1.00	0.005	1.00	-116122.00
GLN100	H	1.00	0.010	1.00	-1129537.00
GLN100	HG2	0.94	0.009	1.00	-108384.00
GLN100	HG3	0.93	0.018	1.00	-79322.00
GLY101	HA2	1.00	0.005	1.00	-721649.00
GLY101	HA3	1.00	0.003	1.00	-1318539.00
GLY101	H	1.00	0.010	1.00	-6976674.00
TYR102	H	1.00	0.004	1.00	-471038.00
TYR102	HA	0.93	0.013	1.00	-379219.00
TYR102	HB2	0.56	0.022	1.00	-108384.00

3.101.3 Detailed Probabilities of GLY101HA2:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN100	1.00	1.00
GLY101	1.00	1.00
TYR102	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
Q100HA	1.00
G101HA3	1.00
G101H	1.00
G101HA2	1.00
Y102HA	1.00
Y102H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN100	HA	1.00	0.005	1.00	0.06
GLN100	HB3	0.63	0.003	1.00	0.06
GLN100	H	0.73	0.010	1.00	-298211.00
GLY101	HA2	1.00	0.006	1.00	2.39
GLY101	HA3	1.00	0.003	1.00	2.25
GLY101	H	1.00	0.005	1.00	-721649.00
TYR102	HA	1.00	0.275	0.00	0.00
TYR102	H	1.00	0.015	1.00	-112268.00

3.101.4 Detailed Probabilities of GLY101HA3:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN100	1.00	1.00
GLY101	1.00	1.00
TYR102	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q100HA	1.00
G101HA2	1.00
G101H	1.00
G101HA3	1.00
Y102HA	1.00
Y102H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN100	HA	1.00	0.002	1.00	0.06
GLN100	HB3	0.72	0.027	1.00	2.70
GLY101	HA2	1.00	0.001	1.00	2.28
GLY101	HA3	1.00	0.001	1.00	4.22
GLY101	H	1.00	0.003	1.00	-1318539.00
TYR102	HA	1.00	0.012	1.00	0.29
TYR102	H	1.00	0.003	1.00	-94994.00

3.101.5 Detailed Probabilities of GLY101H:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN100	0.50	1.00
GLY101	0.67	1.00
TYR102	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q100HB3	1.00
Q100H	1.00
Q100HA	1.00
Q100HB2	1.00
G101HA2	1.00
G101HA3	1.00
G101H	1.00
Y102H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN100	HA	1.00	0.001	1.00	0.29
GLN100	HB2	1.00	0.004	1.00	0.09
GLN100	HB3	1.00	0.151	0.00	0.00
GLN100	H	1.00	0.061	0.00	0.00
GLY101	HA2	1.00	0.001	1.00	0.57
GLY101	HA3	1.00	0.952	0.00	0.00
GLY101	H	1.00	0.010	1.00	-6976674.00
TYR102	H	1.00	0.002	1.00	-281616.00

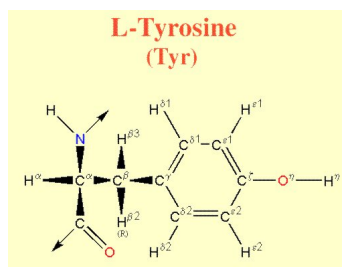
3.102 TYR(102)

Figure 101: Image from the BMRB

Residue probability: 0.841

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.747	175.405	2.122	0.000	0.000
CA 3.102.1	56.254	58.279	6.333	0.333	1.000
CB 3.102.2	39.048	39.527	6.280	0.857	1.000
CD 3.102.3	132.425	132.994	20.285	0.860	1.000
CE1 3.102.4	118.203	117.867	2.496	1.000	1.000
CE2 3.102.5	118.264	117.793	3.050	1.000	1.000
N 3.102.6	117.993	120.136	8.494	0.989	1.000
HA 3.102.7	4.672	4.610	0.592	0.700	1.000
HB2 3.102.8	2.472	2.886	0.452	0.889	1.000
HB3 3.102.9	2.751	2.808	0.478	0.889	1.000
HD 3.102.10	6.984	6.912	0.327	0.986	1.000
HE1 3.102.11	6.716	6.692	0.243	1.000	1.000
HE2 3.102.12	6.716	6.690	0.252	0.800	1.000
H 3.102.13	6.890	8.326	0.740	0.633	1.000
HH	NA	—	—	0.000	0.000

3.102.1 Detailed Probabilities of TYR102CA:

Overall probability: 0.333

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLY101	0.50	1.00
TYR102	0.40	1.00
GLU103	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
G101HA2	1.00
G101HA3	1.00
Y102HB2	1.00
Y102HB3	1.00
Y102HD1	1.00
Y102H	1.00
Y102HA	1.00
E103H	1.00
E103HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLY101	HA2	1.00	0.275	0.00	0.00
GLY101	HA3	1.00	0.012	1.00	0.29
TYR102	HA	1.00	0.006	1.00	3.03
TYR102	HB2	1.00	0.253	0.00	0.00
TYR102	HB3	1.00	0.532	0.00	0.00
TYR102	HD1	1.00	0.015	1.00	0.55
TYR102	H	1.00	0.109	0.00	0.00
GLU103	HA	1.00	0.171	0.00	0.00
GLU103	H	1.00	0.252	0.00	0.00

3.102.2 Detailed Probabilities of TYR102CB:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR102	0.83	1.00
GLU103	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y102HA	1.00
Y102HB3	1.00
Y102HD1	1.00
Y102HE2	1.00
Y102H	1.00
Y102HB2	1.00
E103H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR102	HA	1.00	0.003	1.00	0.22
TYR102	HB2	1.00	0.009	1.00	1.39
TYR102	HB3	1.00	0.002	1.00	0.93
TYR102	HD1	1.00	0.002	1.00	0.33
TYR102	HE2	1.00	0.180	0.00	0.00
TYR102	H	1.00	0.006	1.00	0.16
GLU103	H	1.00	0.010	1.00	0.13

3.102.3 Detailed Probabilities of TYR102CD1:

Overall probability: 0.860

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR102	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
Y102HA	1.00
Y102HB2	1.00
Y102HB3	1.00
Y102HD2	1.00
Y102HE1	1.00
Y102HE2	1.00
Y102H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR102	HA	1.00	0.006	1.00	0.85
TYR102	HB2	1.00	0.004	1.00	0.93
TYR102	HB3	1.00	0.002	1.00	0.91
TYR102	HD1	1.00	0.002	1.00	16.21
TYR102	HE1	1.00	0.004	1.00	3.82
TYR102	HE2	1.00	0.004	1.00	3.82
TYR102	H	0.98	0.096	0.02	0.00

3.102.4 Detailed Probabilities of TYR102CE1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR102	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y102HD1	1.00
Y102HE2	1.00
Y102HE1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR102	HD1	1.00	0.001	1.00	4.46
TYR102	HE1	1.00	0.004	1.00	34.17
TYR102	HE2	1.00	0.004	1.00	34.17
TYR102	HB2	0.89	0.019	1.00	0.20
TYR102	HB3	0.88	0.002	1.00	0.23

3.102.5 Detailed Probabilities of TYR102CE2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR102	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y102HB2	1.00
Y102HB3	1.00
Y102HD1	1.00
Y102HE1	1.00
Y102HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR102	HB2	1.00	0.019	1.00	0.20
TYR102	HB3	1.00	0.002	1.00	0.23
TYR102	HD1	1.00	0.001	1.00	4.46
TYR102	HE1	1.00	0.004	1.00	34.17
TYR102	HE2	1.00	0.004	1.00	34.17

3.102.6 Detailed Probabilities of TYR102N:

Overall probability: 0.989

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLY101	1.00	1.00
TYR102	0.98	1.00
GLU103	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
G101HA2	1.00
G101HA3	1.00
G101H	1.00
Y102HA	1.00
Y102HB2	1.00
Y102HB3	1.00
Y102HD1	1.00
Y102H	1.00
E103H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLY101	HA2	1.00	0.015	1.00	-112268.00
GLY101	HA3	1.00	0.003	1.00	-94994.00
GLY101	H	1.00	0.002	1.00	-281616.00
TYR102	HA	1.00	0.006	1.00	-179732.00
TYR102	HB2	1.00	0.001	1.00	-270311.00
TYR102	HB3	1.00	0.004	1.00	-193154.00
TYR102	HD1	1.00	0.031	0.90	0.00
TYR102	H	1.00	0.003	1.00	-2125002.00
GLU103	H	1.00	0.010	1.00	-85920.00

3.102.7 Detailed Probabilities of TYR102HA:

Overall probability: 0.700

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLY101	0.67	1.00
TYR102	0.80	1.00
GLU103	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
G101HA2	1.00
G101HA3	1.00
Y102HB2	1.00
Y102HB3	1.00
Y102HD1	1.00
Y102H	1.00
Y102HA	1.00
E103H	1.00
E103HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLY101	HA2	1.00	0.002	1.00	0.10
GLY101	HA3	1.00	0.262	0.00	0.00
GLY101	H	0.93	0.013	1.00	-379219.00
TYR102	HA	1.00	0.006	1.00	3.03
TYR102	HB2	1.00	0.003	1.00	0.22
TYR102	HB3	1.00	0.147	0.00	0.00
TYR102	HD1	1.00	0.006	1.00	0.85
TYR102	H	1.00	0.006	1.00	-179732.00
GLU103	HA	1.00	0.131	0.00	0.00
GLU103	H	1.00	0.008	1.00	-784539.00

3.102.8 Detailed Probabilities of TYR102HB2:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR102	0.86	1.00
GLU103	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y102HA	1.00
Y102HB3	1.00
Y102HD1	1.00
Y102HE2	1.00
Y102H	1.00
Y102HB2	1.00
E103H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR102	HA	1.00	0.253	0.00	0.00
TYR102	HB2	1.00	0.009	1.00	1.39
TYR102	HB3	1.00	0.006	1.00	0.96
TYR102	HD1	1.00	0.004	1.00	0.93
TYR102	HE2	1.00	0.019	1.00	0.20
TYR102	H	1.00	0.001	1.00	-270311.00
TYR102	HE1	0.89	0.019	1.00	0.20
GLU103	H	1.00	0.010	1.00	-154270.00
GLU103	HA	0.65	0.008	1.00	0.08

3.102.9 Detailed Probabilities of TYR102HB3:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR102	0.86	1.00
GLU103	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y102HA	1.00
Y102HB2	1.00
Y102HD1	1.00
Y102HE2	1.00
Y102H	1.00
Y102HB3	1.00
E103H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR102	HA	1.00	0.532	0.00	0.00
TYR102	HB2	1.00	0.002	1.00	0.93
TYR102	HB3	1.00	0.024	1.00	14.09
TYR102	HD1	1.00	0.002	1.00	0.91
TYR102	HE2	1.00	0.002	1.00	0.23
TYR102	H	1.00	0.004	1.00	-193154.00
TYR102	HE1	0.88	0.002	1.00	0.23
GLU103	H	1.00	0.001	1.00	-342306.00
GLU103	HA	0.83	0.001	1.00	0.12

3.102.10 Detailed Probabilities of TYR102HD1:

Overall probability: 0.986

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR102	0.99	1.00

Expected NOESY Contacts

Proton	Expected probability
Y102HA	1.00
Y102HB2	1.00
Y102HB3	1.00
Y102HD2	1.00
Y102HE1	1.00
Y102HE2	1.00
Y102H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR102	HA	1.00	0.015	1.00	0.55
TYR102	HB2	1.00	0.002	1.00	0.33
TYR102	HB3	1.00	0.001	1.00	0.44
TYR102	HD1	1.00	0.002	1.00	16.21
TYR102	HE1	1.00	0.001	1.00	4.46
TYR102	HE2	1.00	0.001	1.00	4.46
TYR102	H	0.98	0.031	0.90	0.00

3.102.11 Detailed Probabilities of TYR102HE1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR102	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y102HD1	1.00
Y102HE2	1.00
Y102HE1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR102	HD1	1.00	0.004	1.00	3.82
TYR102	HE1	1.00	0.004	1.00	34.17
TYR102	HE2	1.00	0.004	1.00	34.17
TYR102	HB3	0.88	0.003	1.00	0.07

3.102.12 Detailed Probabilities of TYR102HE2:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR102	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
Y102HB2	1.00
Y102HB3	1.00
Y102HD1	1.00
Y102HE1	1.00
Y102HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR102	HB2	1.00	0.180	0.00	0.00
TYR102	HB3	1.00	0.003	1.00	0.07
TYR102	HD1	1.00	0.004	1.00	3.82
TYR102	HE1	1.00	0.004	1.00	34.17
TYR102	HE2	1.00	0.004	1.00	34.17

3.102.13 Detailed Probabilities of TYR102H:

Overall probability: 0.633

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLY101	1.00	1.00
TYR102	0.40	1.00
GLU103	0.70	1.00

Expected NOESY Contacts

Proton	Expected probability
G101HA2	1.00
G101HA3	1.00
G101H	1.00
Y102HA	1.00
Y102HB2	1.00
Y102HB3	1.00
Y102HD1	1.00
Y102H	1.00
E103H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLY101	HA2	1.00	0.009	1.00	0.14
GLY101	HA3	1.00	0.006	1.00	0.14
GLY101	H	1.00	0.004	1.00	-471038.00
TYR102	HA	1.00	0.109	0.00	0.00
TYR102	HB2	1.00	0.006	1.00	0.16
TYR102	HB3	1.00	0.095	0.00	0.00
TYR102	HD1	1.00	0.096	0.00	0.00
TYR102	H	1.00	0.003	1.00	-2125002.00
GLU103	H	1.00	0.033	0.70	0.00

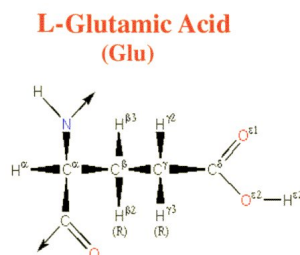
3.103 GLU(103)

Figure 102: Image from the BMRB

Residue probability: 0.666

Residue probability confidence: 0.925

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.162	176.942	2.547	0.000	0.000
CA 3.103.1	56.384	57.442	3.837	0.755	1.000
CB 3.103.2	30.371	30.185	4.018	0.429	0.875
CG 3.103.3	36.249	36.085	1.533	0.714	0.875
N 3.103.4	122.864	120.574	4.837	0.975	1.000
HA 3.103.5	4.507	4.245	0.429	0.900	1.000
HB2 3.103.6	2.087	2.021	0.233	0.571	0.875
HB3 3.103.7	1.987	1.994	0.244	0.571	0.875
HG2 3.103.8	2.256	2.258	0.226	0.286	0.875
HG3 3.103.9	2.323	2.233	0.232	0.571	0.875
H 3.103.10	8.318	8.332	0.601	0.883	1.000
HE2	NA	—	—	0.000	0.000

3.103.1 Detailed Probabilities of GLU103CA:

Overall probability: 0.755

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR102	0.67	1.00
GLU103	0.83	1.00
VAL104	0.65	1.00

Expected NOESY Contacts

Proton	Expected probability
Y102HA	1.00
E103HB2	1.00
E103HB3	1.00
E103HG2	1.00
E103HG3	1.00
E103H	1.00
E103HA	1.00
V104H	1.00
V104HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR102	HA	1.00	0.131	0.00	0.00
TYR102	HB2	0.65	0.008	1.00	0.08
TYR102	HB3	0.83	0.001	1.00	0.12
GLU103	HA	1.00	0.009	1.00	39.72
GLU103	HB2	1.00	0.010	1.00	0.58
GLU103	HB3	1.00	0.003	1.00	0.89
GLU103	HG2	1.00	0.081	0.00	0.00
GLU103	HG3	1.00	0.014	1.00	0.47
GLU103	H	1.00	0.013	1.00	0.39
VAL104	HA	1.00	0.037	0.30	0.00
VAL104	H	1.00	0.003	1.00	2.13

3.103.2 Detailed Probabilities of GLU103CB:

Overall probability: 0.429

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU103	0.50	0.86
VAL104	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E103HA	1.00
E103HB2	1.00
E103HG2	1.00
E103HG3	1.00
E103H	1.00
E103HE2	1.00
E103HB3	1.00
V104H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU103	HA	1.00	0.012	1.00	0.60
GLU103	HB2	1.00	0.129	0.00	0.00
GLU103	HB3	1.00	0.029	1.00	11.43
GLU103	HG2	1.00	0.298	0.00	0.00
GLU103	HG3	1.00	0.351	0.00	0.00
GLU103	H	1.00	0.008	1.00	0.35
VAL104	H	1.00	0.144	0.00	0.00

3.103.3 Detailed Probabilities of GLU103CG:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU103	0.67	0.86
VAL104	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E103HA	1.00
E103HB2	1.00
E103HB3	1.00
E103HG2	1.00
E103H	1.00
E103HE2	1.00
E103HG3	1.00
V104H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU103	HA	1.00	0.006	1.00	0.80
GLU103	HB2	1.00	0.007	1.00	8.87
GLU103	HB3	1.00	0.093	0.00	0.00
GLU103	HG2	1.00	0.176	0.00	0.00
GLU103	HG3	1.00	0.027	1.00	100.68
GLU103	H	1.00	0.011	1.00	0.15
VAL104	H	0.96	0.005	1.00	0.53

3.103.4 Detailed Probabilities of GLU103N:

Overall probability: 0.975

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR102	0.94	1.00
GLU103	1.00	1.00
VAL104	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y102HB3	1.00
Y102HB2	1.00
Y102HA	1.00
Y102H	1.00
E103HA	1.00
E103HB2	1.00
E103HB3	1.00
E103HG2	1.00
E103HG3	1.00
E103H	1.00
V104H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR102	HA	1.00	0.008	1.00	-784539.00
TYR102	HB2	1.00	0.010	1.00	-154270.00
TYR102	HB3	1.00	0.001	1.00	-342306.00
TYR102	H	1.00	0.033	0.70	0.00
TYR102	HD1	0.78	0.002	1.00	-150339.00
GLU103	HA	1.00	0.018	1.00	-463801.00
GLU103	HB2	1.00	0.001	1.00	-377712.00
GLU103	HB3	1.00	0.002	1.00	-418372.00
GLU103	HG2	1.00	0.000	1.00	-82314.00
GLU103	HG3	1.00	0.017	1.00	-71204.00
GLU103	H	1.00	0.014	1.00	-5070981.00
VAL104	H	1.00	0.006	1.00	-137073.00

3.103.5 Detailed Probabilities of GLU103HA:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR102	0.50	1.00
GLU103	1.00	1.00
VAL104	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y102HA	1.00
E103HB2	1.00
E103HB3	1.00
E103HG2	1.00
E103HG3	1.00
E103H	1.00
E103HA	1.00
V104H	1.00
V104HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR102	HA	1.00	0.171	0.00	0.00
TYR102	HB3	0.83	0.018	1.00	0.06
GLU103	HA	1.00	0.009	1.00	39.72
GLU103	HB2	1.00	0.002	1.00	0.90
GLU103	HB3	1.00	0.012	1.00	0.60
GLU103	HG2	1.00	0.012	1.00	0.75
GLU103	HG3	1.00	0.006	1.00	0.80
GLU103	H	1.00	0.018	1.00	-463801.00
VAL104	HA	1.00	0.018	1.00	0.09
VAL104	H	1.00	0.006	1.00	-2376655.00

3.103.6 Detailed Probabilities of GLU103HB2:

Overall probability: 0.571

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU103	0.50	0.86
VAL104	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E103HA	1.00
E103HB3	1.00
E103HG2	1.00
E103HG3	1.00
E103H	1.00
E103HE2	1.00
E103HB2	1.00
V104H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU103	HA	1.00	0.010	1.00	0.58
GLU103	HB2	1.00	0.412	0.00	0.00
GLU103	HB3	1.00	0.129	0.00	0.00
GLU103	HG2	1.00	0.208	0.00	0.00
GLU103	HG3	1.00	0.007	1.00	8.87
GLU103	H	1.00	0.001	1.00	-377712.00
VAL104	H	1.00	0.011	1.00	-219598.00

3.103.7 Detailed Probabilities of GLU103HB3:

Overall probability: 0.571

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU103	0.50	0.86
VAL104	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E103HA	1.00
E103HB2	1.00
E103HG2	1.00
E103HG3	1.00
E103H	1.00
E103HE2	1.00
E103HB3	1.00
V104H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU103	HA	1.00	0.003	1.00	0.89
GLU103	HB2	1.00	0.423	0.00	0.00
GLU103	HB3	1.00	0.029	1.00	11.43
GLU103	HG2	1.00	0.108	0.00	0.00
GLU103	HG3	1.00	0.093	0.00	0.00
GLU103	H	1.00	0.002	1.00	-418372.00
VAL104	H	1.00	0.025	1.00	-790587.00

3.103.8 Detailed Probabilities of GLU103HG2:

Overall probability: 0.286

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU103	0.17	0.86
VAL104	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E103HA	1.00
E103HB2	1.00
E103HB3	1.00
E103HG3	1.00
E103H	1.00
E103HE2	1.00
E103HG2	1.00
V104H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU103	HA	1.00	0.081	0.00	0.00
GLU103	HB2	1.00	0.243	0.00	0.00
GLU103	HB3	1.00	0.298	0.00	0.00
GLU103	HG2	1.00	0.189	0.00	0.00
GLU103	HG3	1.00	0.176	0.00	0.00
GLU103	H	1.00	0.000	1.00	-82314.00
VAL104	H	0.98	0.015	1.00	-166933.00

3.103.9 Detailed Probabilities of GLU103HG3:

Overall probability: 0.571

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU103	0.50	0.86
VAL104	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E103HA	1.00
E103HB2	1.00
E103HB3	1.00
E103HG2	1.00
E103H	1.00
E103HE2	1.00
E103HG3	1.00
V104H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU103	HA	1.00	0.014	1.00	0.47
GLU103	HB2	1.00	0.176	0.00	0.00
GLU103	HB3	1.00	0.351	0.00	0.00
GLU103	HG2	1.00	0.122	0.00	0.00
GLU103	HG3	1.00	0.027	1.00	100.68
GLU103	H	1.00	0.017	1.00	-71204.00
VAL104	H	0.96	0.012	1.00	-289104.00

3.103.10 Detailed Probabilities of GLU103H:

Overall probability: 0.883

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
TYR102	0.72	1.00
GLU103	1.00	1.00
VAL104	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Y102HB3	1.00
Y102HB2	1.00
Y102HA	1.00
Y102H	1.00
E103HA	1.00
E103HB2	1.00
E103HB3	1.00
E103HG2	1.00
E103HG3	1.00
E103H	1.00
V104H	1.00

NOESY contacts detailed probability

3.103 GLU(103)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
TYR102	HA	1.00	0.252	0.00	0.00
TYR102	HB2	1.00	0.010	1.00	0.13
TYR102	HB3	1.00	0.034	0.60	0.00
TYR102	H	1.00	0.010	1.00	-85920.00
TYR102	HD1	0.78	0.019	1.00	0.16
GLU103	HA	1.00	0.013	1.00	0.39
GLU103	HB2	1.00	0.016	1.00	0.41
GLU103	HB3	1.00	0.008	1.00	0.35
GLU103	HG2	1.00	0.011	1.00	0.15
GLU103	HG3	1.00	0.011	1.00	0.15
GLU103	H	1.00	0.014	1.00	-5070981.00
VAL104	H	1.00	0.001	1.00	-129490.00

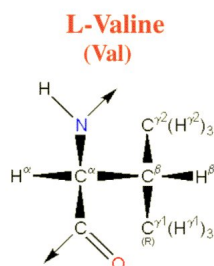


Figure 103: Image from the BMRB

Residue probability: 0.828
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.235	175.682	2.367	0.000	0.000
CA 3.104.1	59.280	62.613	4.828	0.889	1.000
CB 3.104.2	34.167	32.918	4.591	0.833	1.000
CG1 3.104.3	20.686	21.563	2.746	0.757	1.000
CG2 3.104.4	22.008	21.368	2.801	0.800	1.000
N 3.104.5	124.342	121.057	5.832	0.908	1.000
HA 3.104.6	5.228	4.178	0.599	0.788	1.000
HB 3.104.7	1.946	1.980	0.322	1.000	1.000
HG1 3.104.8	0.929	0.816	0.264	0.857	1.000
HG2 3.104.9	0.884	0.803	0.504	0.780	1.000
H 3.104.10	8.651	8.311	0.669	0.667	1.000

3.104.1 Detailed Probabilities of VAL104CA:

Overall probability: 0.889
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU103	1.00	1.00
VAL104	0.80	1.00
ARG105	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E103HA	1.00
V104HG11	1.00
V104HG21	1.00
V104H	1.00
V104HB	1.00
V104HA	1.00
R105HA	1.00
R105H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU103	HA	1.00	0.018	1.00	0.09
VAL104	HA	1.00	0.008	1.00	2.98
VAL104	HB	1.00	0.010	1.00	0.55
VAL104	HG11	1.00	0.026	1.00	0.84
VAL104	HG21	1.00	0.019	1.00	0.84
VAL104	H	1.00	0.047	0.00	0.00
ARG105	HA	1.00	0.004	1.00	0.05
ARG105	H	1.00	0.007	1.00	1.05
ARG105	HB2	0.54	0.013	1.00	0.06

3.104.2 Detailed Probabilities of VAL104CB:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL104	1.00	1.00
ARG105	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V104HA	1.00
V104HG11	1.00
V104HG21	1.00
V104H	1.00
V104HB	1.00
R105H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL104	HA	1.00	0.007	1.00	0.48
VAL104	HB	1.00	0.009	1.00	5.25
VAL104	HG11	1.00	0.023	1.00	1.77
VAL104	HG21	1.00	0.022	1.00	1.77
VAL104	H	1.00	0.009	1.00	0.50
ARG105	H	1.00	0.045	0.00	0.00

3.104.3 Detailed Probabilities of VAL104CG1:

Overall probability: 0.757

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL104	0.80	1.00
ARG105	0.65	1.00

Expected NOESY Contacts

Proton	Expected probability
V104HA	1.00
V104HG12	1.00
V104HG21	1.00
V104H	1.00
V104HB	1.00
R105H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL104	HA	1.00	0.010	1.00	0.76
VAL104	HB	1.00	0.010	1.00	1.81
VAL104	HG11	1.00	0.001	1.00	49.46
VAL104	HG21	1.00	0.046	0.00	0.00
VAL104	H	1.00	0.017	1.00	1.06
ARG105	H	0.98	0.037	0.30	0.00
ARG105	HA	0.56	0.011	1.00	0.13

3.104.4 Detailed Probabilities of VAL104CG2:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL104	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
V104HA	1.00
V104HG11	1.00
V104HG22	1.00
V104H	1.00
V104HB	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL104	HA	1.00	0.008	1.00	0.83
VAL104	HB	1.00	0.008	1.00	3.29
VAL104	HG11	1.00	0.180	0.00	0.00
VAL104	HG21	1.00	0.005	1.00	78.79
VAL104	H	1.00	0.026	1.00	0.77

3.104.5 Detailed Probabilities of VAL104N:

Overall probability: 0.908

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU103	1.00	1.00
VAL104	0.98	1.00
ARG105	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E103HG2	0.98
E103HA	1.00
E103HB2	1.00
E103HG3	0.96
E103HB3	1.00
E103H	1.00
V104HA	1.00
V104HG11	1.00
V104HG21	1.00
V104HB	1.00
V104H	1.00
R105H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU103	HA	1.00	0.006	1.00	-2376655.00
GLU103	HB2	1.00	0.011	1.00	-219598.00
GLU103	HB3	1.00	0.025	1.00	-790587.00
GLU103	HG2	0.98	0.015	1.00	-166933.00
GLU103	HG3	0.96	0.012	1.00	-289104.00
GLU103	H	1.00	0.001	1.00	-129490.00
VAL104	HA	1.00	0.008	1.00	-317702.00
VAL104	HB	1.00	0.016	1.00	-790587.00
VAL104	HG11	1.00	0.014	1.00	-1085721.00
VAL104	HG21	1.00	0.031	0.90	0.00
VAL104	H	1.00	0.003	1.00	-6741406.00
ARG105	H	1.00	0.051	0.00	0.00

3.104.6 Detailed Probabilities of VAL104HA:

Overall probability: 0.788

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU103	0.30	1.00
VAL104	1.00	1.00
ARG105	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E103HA	1.00
V104HG11	1.00
V104HG21	1.00
V104H	1.00
V104HB	1.00
V104HA	1.00
R105HA	1.00
R105H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU103	HA	1.00	0.037	0.30	0.00
VAL104	HA	1.00	0.008	1.00	2.98
VAL104	HB	1.00	0.007	1.00	0.48
VAL104	HG11	1.00	0.010	1.00	0.76
VAL104	HG21	1.00	0.008	1.00	0.83
VAL104	H	1.00	0.008	1.00	-317702.00
ARG105	HA	1.00	0.199	0.00	0.00
ARG105	H	1.00	0.009	1.00	-1752962.00

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
ARG105	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
R105H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL104	HA	1.00	0.010	1.00	0.55
VAL104	HB	1.00	0.009	1.00	5.25
VAL104	HG11	1.00	0.010	1.00	1.81
VAL104	HG21	1.00	0.008	1.00	3.29
VAL104	H	1.00	0.016	1.00	-790587.00
ARG105	H	1.00	0.003	1.00	-249656.00

3.104.8 Detailed Probabilities of VAL104HG11:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL104	0.80	1.00
ARG105	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
R105H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL104	HA	1.00	0.026	1.00	0.84
VAL104	HB	1.00	0.023	1.00	1.77
VAL104	HG11	1.00	0.001	1.00	49.46
VAL104	HG21	1.00	0.180	0.00	0.00
VAL104	H	1.00	0.014	1.00	-1085721.00
ARG105	H	0.98	0.028	1.00	-885981.00
ARG105	HA	0.56	0.025	1.00	0.42

3.104.9 Detailed Probabilities of VAL104HG21:

Overall probability: 0.780

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL104	0.78	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	0.019	1.00	0.84
VAL104	HB	1.00	0.022	1.00	1.77
VAL104	HG11	1.00	0.046	0.00	0.00
VAL104	HG21	1.00	0.005	1.00	78.79
VAL104	H	1.00	0.031	0.90	0.00

3.104.10 Detailed Probabilities of VAL104H:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU103	0.67	1.00
VAL104	0.80	1.00
ARG105	0.00	1.00

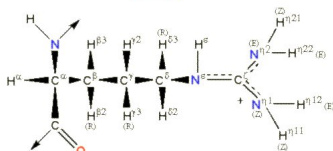
Expected NOESY Contacts

Proton	Expected probability
E103HG2	0.98
E103HA	1.00
E103HB2	1.00
E103HG3	0.96
E103HB3	1.00
E103H	1.00
V104HA	1.00
V104HG11	1.00
V104HG21	1.00
V104HB	1.00
V104H	1.00
R105H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU103	HA	1.00	0.003	1.00	2.13
GLU103	HB2	1.00	0.127	0.00	0.00
GLU103	HB3	1.00	0.144	0.00	0.00
GLU103	HG2	0.98	0.005	1.00	0.53
GLU103	HG3	0.96	0.005	1.00	0.53
GLU103	H	1.00	0.006	1.00	-137073.00
VAL104	HA	1.00	0.047	0.00	0.00
VAL104	HB	1.00	0.009	1.00	0.50
VAL104	HG11	1.00	0.017	1.00	1.06
VAL104	HG21	1.00	0.026	1.00	0.77
VAL104	H	1.00	0.003	1.00	-6741406.00
ARG105	H	1.00	0.051	0.00	0.00

L-Arginine (Arg)



Residue probability: 0.440
Residue probability confidence: 0.911

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	173.917	176.453	2.303	0.000	0.000
CA 3.105.1	52.465	56.803	3.326	0.169	1.000
CB 3.105.2	32.955	30.892	2.424	0.500	1.000
CG 3.105.3	26.576	27.247	1.538	0.444	0.900
CD 3.105.4	41.442	43.189	1.415	0.789	0.800
N 3.105.5	124.856	120.701	3.779	0.725	1.000
NE 3.105.6	82.387	89.115	13.484	0.000	0.778
NH1	NA	–	–	0.000	0.000
NH2	NA	–	–	0.000	0.000
HA 3.105.7	4.915	4.301	0.495	0.750	1.000
HB2 3.105.8	1.857	1.793	0.292	0.000	1.000
HB3 3.105.9	1.816	1.757	0.307	0.233	1.000
HG2 3.105.10	1.805	1.559	0.294	0.337	0.909
HG3 3.105.11	1.752	1.535	0.310	0.150	0.900
HD2 3.105.12	3.515	3.105	0.301	0.717	0.800
HD3 3.105.13	3.339	3.081	0.306	0.714	0.800
H 3.105.14	8.705	8.248	0.623	0.736	1.000
HE 3.105.15	7.599	7.398	0.718	0.333	0.778
HH1	NA	–	–	0.000	0.000
HH2	NA	–	–	0.000	0.000

Overall probability: 0.169
Overall confidence: 1.000

Residue	Probability	Confidence
VAL104	0.50	1.00
ARG105	0.13	1.00
LYS106	0.00	1.00

Residues TOC

Proton	Expected probability
V104HA	1.00
R105HB2	1.00
R105HB3	1.00
R105HG2	1.00
R105HG3	1.00
R105HD2	0.98
R105HD3	0.97
R105H	1.00
R105HA	1.00
K106HA	1.00
K106H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL104	HA	1.00	0.199	0.00	0.00
VAL104	HG11	0.57	0.025	1.00	0.42
ARG105	HA	1.00	0.114	0.00	0.00
ARG105	HB2	1.00	0.198	0.00	0.00
ARG105	HB3	1.00	0.239	0.00	0.00
ARG105	HG2	1.00	0.250	0.00	0.00
ARG105	HG3	1.00	0.303	0.00	0.00
ARG105	HD2	0.98	0.181	0.02	0.00
ARG105	HD3	0.97	0.005	1.00	0.52
ARG105	H	1.00	0.371	0.00	0.00
LYS106	HA	1.00	0.142	0.00	0.00
LYS106	H	1.00	0.377	0.00	0.00

3.105.2 Detailed Probabilities of ARG105CB:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG105	0.44	1.00
LYS106	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R105HA	1.00
R105HB3	1.00
R105HG2	1.00
R105HG3	1.00
R105HD2	1.00
R105HD3	1.00
R105H	1.00
R105HE	1.00
R105HB2	1.00
K106H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG105	HA	1.00	0.006	1.00	0.13
ARG105	HB2	1.00	1.474	0.00	0.00
ARG105	HB3	1.00	1.515	0.00	0.00
ARG105	HG2	1.00	1.526	0.00	0.00
ARG105	HG3	1.00	1.579	0.00	0.00
ARG105	HD2	1.00	0.006	1.00	0.06
ARG105	HD3	1.00	0.008	1.00	0.07
ARG105	H	1.00	0.006	1.00	0.09
ARG105	HE	1.00	0.480	0.00	0.00
LYS106	H	1.00	0.004	1.00	0.15

3.105.3 Detailed Probabilities of ARG105CG:

Overall probability: 0.444

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG105	0.44	0.90

Expected NOESY Contacts

Proton	Expected probability
R105HA	1.00
R105HB2	1.00
R105HB3	1.00
R105HG2	1.00
R105HD2	1.00
R105HD3	1.00
R105H	1.00
R105HE	1.00
R105HH11	1.00
R105HG3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG105	HA	1.00	0.008	1.00	0.11
ARG105	HB2	1.00	0.540	0.00	0.00
ARG105	HB3	1.00	0.499	0.00	0.00
ARG105	HG2	1.00	0.488	0.00	0.00
ARG105	HG3	1.00	0.435	0.00	0.00
ARG105	HD2	1.00	0.003	1.00	0.22
ARG105	HD3	1.00	0.007	1.00	0.17
ARG105	H	1.00	0.004	1.00	0.07
ARG105	HE	1.00	0.471	0.00	0.00

3.105.4 Detailed Probabilities of ARG105CD:

Overall probability: 0.789

Overall confidence: 0.800

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG105	0.79	0.80

Expected NOESY Contacts

Proton	Expected probability
R105HA	0.98
R105HB2	1.00
R105HB3	1.00
R105HG2	1.00
R105HG3	1.00
R105HD3	1.00
R105HE	1.00
R105HH11	1.00
R105HH21	1.00
R105HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG105	HA	0.98	0.003	1.00	0.47
ARG105	HB2	1.00	0.080	0.00	0.00
ARG105	HB3	1.00	0.039	0.10	0.00
ARG105	HG2	1.00	0.028	1.00	0.61
ARG105	HG3	1.00	0.025	1.00	0.61
ARG105	HD2	1.00	0.002	1.00	3.12
ARG105	HD3	1.00	0.005	1.00	2.29
ARG105	HE	1.00	0.012	1.00	0.15
ARG105	H	0.87	0.000	1.00	0.07

3.105.5 Detailed Probabilities of ARG105N:

Overall probability: 0.725

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL104	0.80	1.00
ARG105	0.70	1.00
LYS106	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
V104HG11	0.98
V104H	1.00
V104HB	1.00
V104HA	1.00
R105HA	1.00
R105HB2	1.00
R105HB3	1.00
R105HG2	1.00
R105HG3	1.00
R105H	1.00
K106H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL104	HA	1.00	0.009	1.00	-1752962.00
VAL104	HB	1.00	0.003	1.00	-249656.00
VAL104	HG11	0.98	0.028	1.00	-885981.00
VAL104	H	1.00	0.051	0.00	0.00
VAL104	HG21	0.94	0.017	1.00	-885981.00
ARG105	HA	1.00	0.003	1.00	-249172.00
ARG105	HB2	1.00	0.067	0.00	0.00
ARG105	HB3	1.00	0.026	1.00	-545563.00
ARG105	HG2	1.00	0.015	1.00	-545563.00
ARG105	HG3	1.00	0.038	0.20	0.00
ARG105	H	1.00	0.003	1.00	-4371539.00
LYS106	H	1.00	0.035	0.50	0.00

3.105.6 Detailed Probabilities of ARG105NE:

Overall probability: 0.000

Overall confidence: 0.778

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG105	0.00	0.78

Expected NOESY Contacts

Proton	Expected probability
R105HB2	1.00
R105HB3	1.00
R105HG2	1.00
R105HG3	1.00
R105HD2	1.00
R105HD3	1.00
R105HH11	1.00
R105HH21	1.00
R105HE	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
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3.105.7 Detailed Probabilities of ARG105HA:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL104	1.00	1.00
ARG105	0.75	1.00
LYS106	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
V104HA	1.00
R105HB2	1.00
R105HB3	1.00
R105HG2	1.00
R105HG3	1.00
R105HD2	0.98
R105HD3	0.97
R105H	1.00
R105HA	1.00
K106HA	1.00
K106H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL104	HA	1.00	0.004	1.00	0.05
VAL104	HG11	0.57	0.011	1.00	0.13
ARG105	HA	1.00	0.114	0.00	0.00
ARG105	HB2	1.00	0.006	1.00	0.13
ARG105	HB3	1.00	0.005	1.00	0.14
ARG105	HG2	1.00	1.400	0.00	0.00
ARG105	HG3	1.00	0.008	1.00	0.11
ARG105	HD2	0.98	0.003	1.00	0.47
ARG105	HD3	0.97	0.003	1.00	0.60
ARG105	H	1.00	0.003	1.00	-249172.00
LYS106	HA	1.00	0.279	0.00	0.00
LYS106	H	1.00	0.003	1.00	-1553448.00

3.105.8 Detailed Probabilities of ARG105HB2:

Overall probability: 0.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG105	0.00	1.00
LYS106	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R105HA	1.00
R105HB3	1.00
R105HG2	1.00
R105HG3	1.00
R105HD2	1.00
R105HD3	1.00
R105H	1.00
R105HE	1.00
R105HB2	1.00
K106H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG105	HA	1.00	0.198	0.00	0.00
ARG105	HB2	1.00	1.474	0.00	0.00
ARG105	HB3	1.00	1.066	0.00	0.00
ARG105	HG2	1.00	1.472	0.00	0.00
ARG105	HG3	1.00	0.540	0.00	0.00
ARG105	HD2	1.00	0.080	0.00	0.00
ARG105	HD3	1.00	0.058	0.00	0.00
ARG105	H	1.00	0.067	0.00	0.00
LYS106	H	1.00	0.145	0.00	0.00

3.105.9 Detailed Probabilities of ARG105HB3:

Overall probability: 0.233

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG105	0.26	1.00
LYS106	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R105HA	1.00
R105HB2	1.00
R105HG2	1.00
R105HG3	1.00
R105HD2	1.00
R105HD3	1.00
R105H	1.00
R105HE	1.00
R105HB3	1.00
K106H	1.00

NOESY contacts detailed probability

3.105 ARG(105)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG105	HA	1.00	0.239	0.00	0.00
ARG105	HB2	1.00	1.515	0.00	0.00
ARG105	HB3	1.00	1.025	0.00	0.00
ARG105	HG2	1.00	1.513	0.00	0.00
ARG105	HG3	1.00	0.499	0.00	0.00
ARG105	HD2	1.00	0.039	0.10	0.00
ARG105	HD3	1.00	0.017	1.00	0.60
ARG105	H	1.00	0.026	1.00	-545563.00
LYS106	H	1.00	0.104	0.00	0.00

3.105.10 Detailed Probabilities of ARG105HG2:

Overall probability: 0.337

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG105	0.38	0.90
LYS106	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
R105HA	1.00
R105HB2	1.00
R105HB3	1.00
R105HG3	1.00
R105HD2	1.00
R105HD3	1.00
R105H	1.00
R105HE	1.00
R105HH11	1.00
R105HG2	1.00
K106H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG105	HA	1.00	0.250	0.00	0.00
ARG105	HB2	1.00	1.526	0.00	0.00
ARG105	HB3	1.00	1.014	0.00	0.00
ARG105	HG2	1.00	1.524	0.00	0.00
ARG105	HG3	1.00	0.488	0.00	0.00
ARG105	HD2	1.00	0.028	1.00	0.61
ARG105	HD3	1.00	0.006	1.00	0.60
ARG105	H	1.00	0.015	1.00	-545563.00
LYS106	H	0.97	0.093	0.03	0.00

3.105.11 Detailed Probabilities of ARG105HG3:

Overall probability: 0.150

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG105	0.15	0.90

Expected NOESY Contacts

Proton	Expected probability
R105HA	1.00
R105HB2	1.00
R105HB3	1.00
R105HG2	1.00
R105HD2	1.00
R105HD3	1.00
R105H	1.00
R105HE	1.00
R105HH11	1.00
R105HG3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG105	HA	1.00	0.303	0.00	0.00
ARG105	HB2	1.00	1.579	0.00	0.00
ARG105	HB3	1.00	0.961	0.00	0.00
ARG105	HG2	1.00	1.577	0.00	0.00
ARG105	HG3	1.00	0.435	0.00	0.00
ARG105	HD2	1.00	0.025	1.00	0.61
ARG105	HD3	1.00	0.047	0.00	0.00
ARG105	H	1.00	0.038	0.20	0.00

3.105.12 Detailed Probabilities of ARG105HD2:

Overall probability: 0.717

Overall confidence: 0.800

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG105	0.72	0.80

Expected NOESY Contacts

Proton	Expected probability
R105HA	0.98
R105HB2	1.00
R105HB3	1.00
R105HG2	1.00
R105HG3	1.00
R105HD3	1.00
R105HE	1.00
R105HH11	1.00
R105HH21	1.00
R105HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG105	HA	0.98	0.181	0.02	0.00
ARG105	HB2	1.00	0.006	1.00	0.06
ARG105	HB3	1.00	0.722	0.00	0.00
ARG105	HG2	1.00	0.000	1.00	0.22
ARG105	HG3	1.00	0.003	1.00	0.22
ARG105	HD2	1.00	0.002	1.00	3.12
ARG105	HD3	1.00	0.001	1.00	2.30

3.105.13 Detailed Probabilities of ARG105HD3:

Overall probability: 0.714

Overall confidence: 0.800

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG105	0.71	0.80

Expected NOESY Contacts

Proton	Expected probability
R105HA	0.97
R105HB2	1.00
R105HB3	1.00
R105HG2	1.00
R105HG3	1.00
R105HD2	1.00
R105HE	1.00
R105HH11	1.00
R105HH21	1.00
R105HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG105	HA	0.97	0.005	1.00	0.52
ARG105	HB2	1.00	0.008	1.00	0.07
ARG105	HB3	1.00	0.898	0.00	0.00
ARG105	HG2	1.00	0.010	1.00	0.21
ARG105	HG3	1.00	0.007	1.00	0.17
ARG105	HD2	1.00	0.005	1.00	2.29
ARG105	HD3	1.00	0.177	0.00	0.00

3.105.14 Detailed Probabilities of ARG105H:

Overall probability: 0.736

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL104	0.46	1.00
ARG105	0.88	1.00
LYS106	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V104HG11	0.98
V104H	1.00
V104HB	1.00
V104HA	1.00
R105HA	1.00
R105HB2	1.00
R105HB3	1.00
R105HG2	1.00
R105HG3	1.00
R105H	1.00
K106H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL104	HA	1.00	0.007	1.00	1.05
VAL104	HB	1.00	0.045	0.00	0.00
VAL104	HG11	0.98	0.037	0.30	0.00
VAL104	H	1.00	0.051	0.00	0.00
VAL104	HG21	0.94	0.028	1.00	0.77
ARG105	HA	1.00	0.371	0.00	0.00
ARG105	HB2	1.00	0.006	1.00	0.09
ARG105	HB3	1.00	0.003	1.00	0.08
ARG105	HG2	1.00	0.012	1.00	0.06
ARG105	HG3	1.00	0.004	1.00	0.07
ARG105	H	1.00	0.003	1.00	-4371539.00
ARG105	HD2	0.87	0.000	1.00	0.07
ARG105	HD3	0.86	0.001	1.00	0.08
LYS106	H	1.00	0.016	1.00	-107133.00

3.105.15 Detailed Probabilities of ARG105HE:

Overall probability: 0.333

Overall confidence: 0.778

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG105	0.33	0.78

Expected NOESY Contacts

Proton	Expected probability
R105HB2	1.00
R105HB3	1.00
R105HG2	1.00
R105HG3	1.00
R105HD2	1.00
R105HD3	1.00
R105HH11	1.00
R105HH21	1.00
R105HE	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG105	HB2	1.00	0.480	0.00	0.00
ARG105	HB3	1.00	0.453	0.00	0.00
ARG105	HG2	1.00	0.459	0.00	0.00
ARG105	HG3	1.00	0.471	0.00	0.00
ARG105	HD2	1.00	0.012	1.00	0.15
ARG105	HD3	1.00	0.012	1.00	0.13

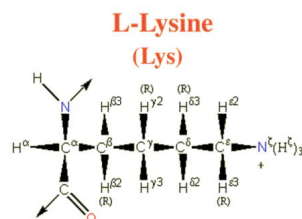


Figure 105: Image from the BMRB

Residue probability: 0.555
Residue probability confidence: 0.945

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.820	176.660	3.133	0.000	0.000
CA 3.106.1	53.868	57.014	3.028	0.512	1.000
CB 3.106.2	35.299	32.981	3.186	0.917	1.000
CG 3.106.3	24.003	24.941	1.956	0.273	0.917
CD 3.106.4	29.231	29.020	2.193	0.302	0.900
CE 3.106.5	41.780	41.893	1.492	0.862	0.889
N 3.106.6	121.499	120.954	4.210	0.464	1.000
NZ	NA	—	—	0.000	0.000
HA 3.106.7	5.578	4.262	0.489	0.670	1.000
HB2 3.106.8	1.716	1.774	0.365	0.636	1.000
HB3 3.106.9	1.714	1.742	0.385	0.636	1.000
HG2 3.106.10	1.460	1.358	0.344	0.436	0.917
HG3 3.106.11	1.402	1.343	0.357	0.273	0.917
HD2 3.106.12	1.561	1.614	0.957	0.447	0.900
HD3 3.106.13	1.562	1.595	0.387	0.447	0.900
HE2 3.106.14	2.952	2.907	0.230	0.650	0.889
HE3 3.106.15	2.953	2.901	0.241	0.650	0.889
H 3.106.16	8.807	8.185	0.605	0.702	1.000
HZ	NA	—	—	0.000	0.000

3.106.1 Detailed Probabilities of LYS106CA:

Overall probability: 0.512
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG105	0.00	1.00
LYS106	0.52	1.00
VAL107	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
R105HA	1.00
K106HB2	1.00
K106HB3	1.00
K106HG2	1.00
K106HG3	1.00
K106HD2	0.98
K106HD3	0.98
K106H	1.00
K106HA	1.00
V107HA	1.00
V107H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG105	HA	1.00	0.279	0.00	0.00
LYS106	HA	1.00	0.012	1.00	3.39
LYS106	HB2	1.00	0.006	1.00	0.92
LYS106	HB3	1.00	0.008	1.00	0.92
LYS106	HG2	1.00	0.007	1.00	0.52
LYS106	HG3	1.00	0.065	0.00	0.00
LYS106	HD2	0.98	0.094	0.02	0.00
LYS106	HD3	0.98	0.095	0.02	0.00
LYS106	H	1.00	0.039	0.10	0.00
VAL107	HA	1.00	0.579	0.00	0.00
VAL107	H	1.00	0.008	1.00	0.98
VAL107	HG21	0.50	0.013	1.00	0.33

3.106.2 Detailed Probabilities of LYS106CB:

Overall probability: 0.917

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS106	0.90	1.00
VAL107	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K106HA	1.00
K106HB2	1.00
K106HG2	1.00
K106HG3	1.00
K106HD2	1.00
K106HD3	1.00
K106HE2	0.99
K106HE3	0.99
K106H	1.00
K106HB3	1.00
V107H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS106	HA	1.00	0.004	1.00	0.48
LYS106	HB2	1.00	0.003	1.00	4.27
LYS106	HB3	1.00	0.001	1.00	4.27
LYS106	HG2	1.00	0.003	1.00	0.47
LYS106	HG3	1.00	0.061	0.00	0.00
LYS106	HD2	1.00	0.025	1.00	0.36
LYS106	HD3	1.00	0.024	1.00	0.36
LYS106	HE2	0.99	0.016	1.00	0.16
LYS106	HE3	0.99	0.015	1.00	0.16
LYS106	H	1.00	0.012	1.00	0.26
VAL107	H	1.00	0.007	1.00	0.23
VAL107	HA	0.85	0.004	1.00	0.05

3.106.3 Detailed Probabilities of LYS106CG:

Overall probability: 0.273

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS106	0.20	0.91
VAL107	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K106HA	1.00
K106HB2	1.00
K106HB3	1.00
K106HG3	1.00
K106HD2	1.00
K106HD3	1.00
K106HE2	1.00
K106HE3	1.00
K106H	1.00
K106HZ2	1.00
K106HG2	1.00
V107H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS106	HA	1.00	0.002	1.00	0.16
LYS106	HB2	1.00	0.444	0.00	0.00
LYS106	HB3	1.00	0.442	0.00	0.00
LYS106	HG2	1.00	0.188	0.00	0.00
LYS106	HG3	1.00	0.130	0.00	0.00
LYS106	HD2	1.00	0.289	0.00	0.00
LYS106	HD3	1.00	0.290	0.00	0.00
LYS106	HE2	1.00	1.680	0.00	0.00
LYS106	HE3	1.00	1.681	0.00	0.00
LYS106	H	1.00	0.013	1.00	0.22
VAL107	H	0.98	0.029	1.00	0.06

3.106.4 Detailed Probabilities of LYS106CD:

Overall probability: 0.302

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS106	0.30	0.90

Expected NOESY Contacts

Proton	Expected probability
K106HA	0.98
K106HB2	1.00
K106HB3	1.00
K106HG2	1.00
K106HG3	1.00
K106HD2	1.00
K106HE2	1.00
K106HE3	1.00
K106HZ2	1.00
K106HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS106	HA	0.98	2.114	0.02	0.00
LYS106	HB2	1.00	0.368	0.00	0.00
LYS106	HB3	1.00	0.370	0.00	0.00
LYS106	HG2	1.00	0.185	0.00	0.00
LYS106	HG3	1.00	0.127	0.00	0.00
LYS106	HD2	1.00	0.286	0.00	0.00
LYS106	HD3	1.00	0.287	0.00	0.00
LYS106	HE2	1.00	0.006	1.00	0.75
LYS106	HE3	1.00	0.005	1.00	0.75
LYS106	H	0.87	0.006	1.00	0.09

3.106.5 Detailed Probabilities of LYS106CE:

Overall probability: 0.862

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS106	0.86	0.89

Expected NOESY Contacts

Proton	Expected probability
K106HB2	0.98
K106HB3	0.99
K106HG2	1.00
K106HG3	1.00
K106HD2	1.00
K106HD3	1.00
K106HE3	1.00
K106HZ2	1.00
K106HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS106	HB2	0.99	0.020	1.00	15.02
LYS106	HB3	0.99	0.018	1.00	15.02
LYS106	HG2	1.00	0.032	0.80	0.00
LYS106	HG3	1.00	0.009	1.00	1.85
LYS106	HD2	1.00	0.001	1.00	1.96
LYS106	HD3	1.00	0.002	1.00	1.96
LYS106	HE2	1.00	0.035	0.50	0.00
LYS106	HE3	1.00	0.034	0.60	0.00

3.106.6 Detailed Probabilities of LYS106N:

Overall probability: 0.464

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG105	0.51	1.00
LYS106	0.50	1.00
VAL107	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R105HG2	0.97
R105HA	1.00
R105H	1.00
R105HB3	1.00
R105HB2	1.00
K106HA	1.00
K106HB2	1.00
K106HB3	1.00
K106HG2	1.00
K106HG3	1.00
K106H	1.00
V107H	1.00

NOESY contacts detailed probability

3.106 LYS(106)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG105	HA	1.00	0.003	1.00	-1553448.00
ARG105	HB2	1.00	0.145	0.00	0.00
ARG105	HB3	1.00	0.104	0.00	0.00
ARG105	HG2	0.97	0.093	0.03	0.00
ARG105	H	1.00	0.016	1.00	-107133.00
ARG105	HD2	0.55	0.002	1.00	-113214.00
LYS106	HA	1.00	0.005	1.00	-387614.00
LYS106	HB2	1.00	0.004	1.00	-868209.00
LYS106	HB3	1.00	0.002	1.00	-868209.00
LYS106	HG2	1.00	0.252	0.00	0.00
LYS106	HG3	1.00	0.310	0.00	0.00
LYS106	H	1.00	0.118	0.00	0.00
VAL107	H	1.00	0.134	0.00	0.00

3.106.7 Detailed Probabilities of LYS106HA:

Overall probability: 0.670

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG105	0.00	1.00
LYS106	0.75	1.00
VAL107	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
R105HA	1.00
K106HB2	1.00
K106HB3	1.00
K106HG2	1.00
K106HG3	1.00
K106HD2	0.98
K106HD3	0.98
K106H	1.00
K106HA	1.00
V107HA	1.00
V107H	1.00

NOESY contacts detailed probability

3.106 LYS(106)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG105	HA	1.00	0.142	0.00	0.00
LYS106	HA	1.00	0.012	1.00	3.39
LYS106	HB2	1.00	0.004	1.00	0.48
LYS106	HB3	1.00	0.004	1.00	0.48
LYS106	HG2	1.00	0.002	1.00	0.16
LYS106	HG3	1.00	0.003	1.00	0.18
LYS106	HD2	0.98	2.114	0.02	0.00
LYS106	HD3	0.98	2.114	0.02	0.00
LYS106	H	1.00	0.005	1.00	-387614.00
VAL107	HA	1.00	0.082	0.00	0.00
VAL107	H	1.00	0.001	1.00	-1943799.00
VAL107	HG21	0.50	0.002	1.00	0.17

3.106.8 Detailed Probabilities of LYS106HB2:

Overall probability: 0.636

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS106	0.60	1.00
VAL107	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K106HA	1.00
K106HB3	1.00
K106HG2	1.00
K106HG3	1.00
K106HD2	1.00
K106HD3	1.00
K106HE2	0.98
K106HE3	0.99
K106H	1.00
K106HB2	1.00
V107H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS106	HA	1.00	0.006	1.00	0.92
LYS106	HB2	1.00	0.003	1.00	4.27
LYS106	HB3	1.00	0.003	1.00	4.27
LYS106	HG2	1.00	0.444	0.00	0.00
LYS106	HG3	1.00	0.822	0.00	0.00
LYS106	HD2	1.00	0.368	0.00	0.00
LYS106	HD3	1.00	0.368	0.00	0.00
LYS106	HE2	0.98	0.020	1.00	15.02
LYS106	HE3	0.99	0.020	1.00	15.02
LYS106	H	1.00	0.004	1.00	-868209.00
VAL107	H	1.00	0.002	1.00	-866117.00

3.106.9 Detailed Probabilities of LYS106HB3:

Overall probability: 0.636

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS106	0.60	1.00
VAL107	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K106HA	1.00
K106HB2	1.00
K106HG2	1.00
K106HG3	1.00
K106HD2	1.00
K106HD3	1.00
K106HE2	0.99
K106HE3	0.99
K106H	1.00
K106HB3	1.00
V107H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS106	HA	1.00	0.008	1.00	0.92
LYS106	HB2	1.00	0.001	1.00	4.27
LYS106	HB3	1.00	0.001	1.00	4.27
LYS106	HG2	1.00	0.442	0.00	0.00
LYS106	HG3	1.00	0.820	0.00	0.00
LYS106	HD2	1.00	0.370	0.00	0.00
LYS106	HD3	1.00	0.370	0.00	0.00
LYS106	HE2	0.99	0.018	1.00	15.02
LYS106	HE3	0.99	0.018	1.00	15.02
LYS106	H	1.00	0.002	1.00	-868209.00
VAL107	H	1.00	0.004	1.00	-866117.00

3.106.10 Detailed Probabilities of LYS106HG2:

Overall probability: 0.436

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS106	0.46	0.91
VAL107	0.20	1.00

Expected NOESY Contacts

Proton	Expected probability
K106HA	1.00
K106HB2	1.00
K106HB3	1.00
K106HG3	1.00
K106HD2	1.00
K106HD3	1.00
K106HE2	1.00
K106HE3	1.00
K106H	1.00
K106HZ2	1.00
K106HG2	1.00
V107H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS106	HA	1.00	0.007	1.00	0.52
LYS106	HB2	1.00	0.003	1.00	0.47
LYS106	HB3	1.00	0.003	1.00	0.47
LYS106	HG2	1.00	0.188	0.00	0.00
LYS106	HG3	1.00	0.566	0.00	0.00
LYS106	HD2	1.00	0.185	0.00	0.00
LYS106	HD3	1.00	0.185	0.00	0.00
LYS106	HE2	1.00	0.032	0.80	0.00
LYS106	HE3	1.00	0.032	0.80	0.00
LYS106	H	1.00	0.252	0.00	0.00
VAL107	H	0.98	0.038	0.20	0.00

3.106.11 Detailed Probabilities of LYS106HG3:

Overall probability: 0.273

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS106	0.20	0.91
VAL107	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K106HA	1.00
K106HB2	1.00
K106HB3	1.00
K106HG2	1.00
K106HD2	1.00
K106HD3	1.00
K106HE2	1.00
K106HE3	1.00
K106H	1.00
K106HZ2	1.00
K106HG3	1.00
V107H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS106	HA	1.00	0.065	0.00	0.00
LYS106	HB2	1.00	0.061	0.00	0.00
LYS106	HB3	1.00	0.061	0.00	0.00
LYS106	HG2	1.00	0.130	0.00	0.00
LYS106	HG3	1.00	0.508	0.00	0.00
LYS106	HD2	1.00	0.127	0.00	0.00
LYS106	HD3	1.00	0.127	0.00	0.00
LYS106	HE2	1.00	0.009	1.00	1.85
LYS106	HE3	1.00	0.009	1.00	1.85
LYS106	H	1.00	0.310	0.00	0.00
VAL107	H	0.96	0.020	1.00	-336648.00

3.106.12 Detailed Probabilities of LYS106HD2:

Overall probability: 0.447

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS106	0.45	0.90

Expected NOESY Contacts

Proton	Expected probability
K106HA	0.98
K106HB2	1.00
K106HB3	1.00
K106HG2	1.00
K106HG3	1.00
K106HD3	1.00
K106HE2	1.00
K106HE3	1.00
K106HZ2	1.00
K106HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS106	HA	0.98	0.094	0.02	0.00
LYS106	HB2	1.00	0.025	1.00	0.36
LYS106	HB3	1.00	0.025	1.00	0.36
LYS106	HG2	1.00	0.289	0.00	0.00
LYS106	HG3	1.00	0.667	0.00	0.00
LYS106	HD2	1.00	0.286	0.00	0.00
LYS106	HD3	1.00	0.286	0.00	0.00
LYS106	HE2	1.00	0.001	1.00	1.96
LYS106	HE3	1.00	0.001	1.00	1.96

3.106.13 Detailed Probabilities of LYS106HD3:

Overall probability: 0.447

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS106	0.45	0.90

Expected NOESY Contacts

Proton	Expected probability
K106HA	0.98
K106HB2	1.00
K106HB3	1.00
K106HG2	1.00
K106HG3	1.00
K106HD2	1.00
K106HE2	1.00
K106HE3	1.00
K106HZ2	1.00
K106HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS106	HA	0.98	0.095	0.02	0.00
LYS106	HB2	1.00	0.024	1.00	0.36
LYS106	HB3	1.00	0.024	1.00	0.36
LYS106	HG2	1.00	0.290	0.00	0.00
LYS106	HG3	1.00	0.668	0.00	0.00
LYS106	HD2	1.00	0.287	0.00	0.00
LYS106	HD3	1.00	0.287	0.00	0.00
LYS106	HE2	1.00	0.002	1.00	1.96
LYS106	HE3	1.00	0.002	1.00	1.96

3.106.14 Detailed Probabilities of LYS106HE2:

Overall probability: 0.650

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS106	0.65	0.89

Expected NOESY Contacts

Proton	Expected probability
K106HB2	0.98
K106HB3	0.99
K106HG2	1.00
K106HG3	1.00
K106HD2	1.00
K106HD3	1.00
K106HE3	1.00
K106HZ2	1.00
K106HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS106	HB2	0.99	0.015	1.00	0.16
LYS106	HB3	0.99	0.015	1.00	0.16
LYS106	HG2	1.00	1.681	0.00	0.00
LYS106	HG3	1.00	2.059	0.00	0.00
LYS106	HD2	1.00	0.005	1.00	0.75
LYS106	HD3	1.00	0.005	1.00	0.75
LYS106	HE2	1.00	0.034	0.60	0.00
LYS106	HE3	1.00	0.034	0.60	0.00

3.106.15 Detailed Probabilities of LYS106HE3:

Overall probability: 0.650

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS106	0.65	0.89

Expected NOESY Contacts

Proton	Expected probability
K106HB2	0.99
K106HB3	0.99
K106HG2	1.00
K106HG3	1.00
K106HD2	1.00
K106HD3	1.00
K106HE2	1.00
K106HZ2	1.00
K106HE3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS106	HB2	0.99	0.015	1.00	0.16
LYS106	HB3	0.99	0.015	1.00	0.16
LYS106	HG2	1.00	1.681	0.00	0.00
LYS106	HG3	1.00	2.059	0.00	0.00
LYS106	HD2	1.00	0.005	1.00	0.75
LYS106	HD3	1.00	0.005	1.00	0.75
LYS106	HE2	1.00	0.034	0.60	0.00
LYS106	HE3	1.00	0.034	0.60	0.00

3.106.16 Detailed Probabilities of LYS106H:

Overall probability: 0.702

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG105	0.69	1.00
LYS106	0.76	1.00
VAL107	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
R105HG2	0.97
R105HA	1.00
R105H	1.00
R105HB3	1.00
R105HB2	1.00
K106HA	1.00
K106HB2	1.00
K106HB3	1.00
K106HG2	1.00
K106HG3	1.00
K106H	1.00
V107H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG105	HA	1.00	0.377	0.00	0.00
ARG105	HB2	1.00	0.004	1.00	0.15
ARG105	HB3	1.00	0.004	1.00	0.10
ARG105	HG2	0.97	0.114	0.03	0.00
ARG105	H	1.00	0.035	0.50	0.00
ARG105	HG3	0.95	0.011	1.00	0.07
ARG105	HD2	0.55	0.008	1.00	0.18
ARG105	HD3	0.57	0.011	1.00	0.21
LYS106	HA	1.00	0.039	0.10	0.00
LYS106	HB2	1.00	0.012	1.00	0.26
LYS106	HB3	1.00	0.012	1.00	0.26
LYS106	HG2	1.00	0.013	1.00	0.22
LYS106	HG3	1.00	0.014	1.00	0.23
LYS106	H	1.00	0.118	0.00	0.00
LYS106	HD2	0.88	0.006	1.00	0.09
LYS106	HD3	0.87	0.006	1.00	0.09
VAL107	H	1.00	0.581	0.00	0.00
VAL107	HA	0.92	0.013	1.00	0.14

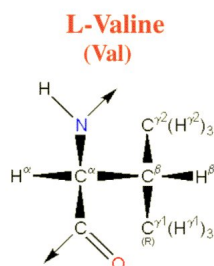


Figure 106: Image from the BMRB

Residue probability: 0.732
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	173.332	175.682	2.367	0.000	0.000
CA 3.107.1	60.222	62.613	4.828	0.660	1.000
CB 3.107.2	35.234	32.918	4.591	0.857	1.000
CG1 3.107.3	21.723	21.563	2.746	0.833	1.000
CG2 3.107.4	20.759	21.368	2.801	0.800	1.000
N 3.107.5	118.792	121.057	5.832	0.485	1.000
HA 3.107.6	4.615	4.178	0.599	0.710	1.000
HB 3.107.7	2.116	1.980	0.322	1.000	1.000
HG1 3.107.8	0.763	0.816	0.264	0.667	1.000
HG2 3.107.9	0.868	0.803	0.504	0.800	1.000
H 3.107.10	8.555	8.311	0.669	0.504	1.000

3.107.1 Detailed Probabilities of VAL107CA:

Overall probability: 0.660
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS106	0.50	1.00
VAL107	0.80	1.00
THR108	0.53	1.00

Expected NOESY Contacts

Proton	Expected probability
K106HA	1.00
V107HG11	1.00
V107HG21	1.00
V107H	1.00
V107HB	1.00
V107HA	1.00
T108H	1.00
T108HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS106	HA	1.00	0.082	0.00	0.00
LYS106	H	0.92	0.013	1.00	0.14
VAL107	HA	1.00	0.007	1.00	6.35
VAL107	HB	1.00	0.004	1.00	1.02
VAL107	HG11	1.00	0.002	1.00	0.92
VAL107	HG21	1.00	0.001	1.00	1.18
VAL107	H	1.00	0.051	0.00	0.00
THR108	HA	1.00	0.159	0.00	0.00
THR108	H	1.00	0.002	1.00	1.70
THR108	HB	0.53	0.034	0.60	0.00

3.107.2 Detailed Probabilities of VAL107CB:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL107	0.80	1.00
THR108	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V107HA	1.00
V107HG11	1.00
V107HG21	1.00
V107H	1.00
V107HB	1.00
T108H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL107	HA	1.00	0.010	1.00	0.62
VAL107	HB	1.00	0.007	1.00	17.61
VAL107	HG11	1.00	0.003	1.00	1.81
VAL107	HG21	1.00	0.002	1.00	1.24
VAL107	H	1.00	0.046	0.00	0.00
THR108	H	1.00	0.003	1.00	0.37
THR108	HA	0.79	0.016	1.00	0.09

3.107.3 Detailed Probabilities of VAL107CG1:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL107	1.00	1.00
THR108	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V107HA	1.00
V107HG12	1.00
V107HG21	1.00
V107H	1.00
V107HB	1.00
T108H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL107	HA	1.00	0.004	1.00	0.73
VAL107	HB	1.00	0.002	1.00	2.40
VAL107	HG11	1.00	0.003	1.00	66.32
VAL107	HG21	1.00	0.004	1.00	5.90
VAL107	H	1.00	0.009	1.00	0.61
THR108	H	0.97	0.040	0.00	0.00

3.107.4 Detailed Probabilities of VAL107CG2:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL107	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
V107HA	1.00
V107HG11	1.00
V107HG22	1.00
V107H	1.00
V107HB	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL107	HA	1.00	0.006	1.00	0.88
VAL107	HB	1.00	0.001	1.00	2.60
VAL107	HG11	1.00	0.104	0.00	0.00
VAL107	HG21	1.00	0.001	1.00	51.68
VAL107	H	1.00	0.026	1.00	1.01

3.107.5 Detailed Probabilities of VAL107N:

Overall probability: 0.485

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS106	0.70	1.00
VAL107	0.22	1.00
THR108	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K106HG2	0.98
K106HG3	0.96
K106HA	1.00
K106HB3	1.00
K106HB2	1.00
K106H	1.00
V107HA	1.00
V107HG11	1.00
V107HG21	1.00
V107HB	1.00
V107H	1.00
T108H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS106	HA	1.00	0.001	1.00	-1943799.00
LYS106	HB2	1.00	0.002	1.00	-866117.00
LYS106	HB3	1.00	0.004	1.00	-866117.00
LYS106	HG2	0.98	0.038	0.20	0.00
LYS106	HG3	0.96	0.020	1.00	-336648.00
LYS106	H	1.00	0.581	0.00	0.00
VAL107	HA	1.00	0.039	0.10	0.00
VAL107	HB	1.00	0.019	1.00	-571030.00
VAL107	HG11	1.00	1.079	0.00	0.00
VAL107	HG21	1.00	0.974	0.00	0.00
VAL107	H	1.00	0.329	0.00	0.00
THR108	H	1.00	0.378	0.00	0.00
THR108	HA	0.91	0.019	1.00	-747524.00

3.107.6 Detailed Probabilities of VAL107HA:

Overall probability: 0.710

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS106	0.67	1.00
VAL107	0.82	1.00
THR108	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
K106HA	1.00
V107HG11	1.00
V107HG21	1.00
V107H	1.00
V107HB	1.00
V107HA	1.00
T108H	1.00
T108HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS106	HA	1.00	0.579	0.00	0.00
LYS106	HB2	0.62	0.004	1.00	0.05
LYS106	HB3	0.85	0.004	1.00	0.05
VAL107	HA	1.00	0.007	1.00	6.35
VAL107	HB	1.00	0.010	1.00	0.62
VAL107	HG11	1.00	0.004	1.00	0.73
VAL107	HG21	1.00	0.006	1.00	0.88
VAL107	H	1.00	0.039	0.10	0.00
THR108	HA	1.00	0.160	0.00	0.00
THR108	H	1.00	0.005	1.00	-1467072.00

3.107.7 Detailed Probabilities of VAL107HB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL107	1.00	1.00
THR108	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V107HA	1.00
V107HG11	1.00
V107HG21	1.00
V107H	1.00
V107HB	1.00
T108H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL107	HA	1.00	0.004	1.00	1.02
VAL107	HB	1.00	0.007	1.00	17.61
VAL107	HG11	1.00	0.002	1.00	2.40
VAL107	HG21	1.00	0.001	1.00	2.60
VAL107	H	1.00	0.019	1.00	-571030.00
THR108	H	1.00	0.002	1.00	-658821.00

3.107.8 Detailed Probabilities of VAL107HG11:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL107	0.60	1.00
THR108	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V107HA	1.00
V107HG12	1.00
V107HG21	1.00
V107H	1.00
V107HB	1.00
T108H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL107	HA	1.00	0.002	1.00	0.92
VAL107	HB	1.00	0.003	1.00	1.81
VAL107	HG11	1.00	0.003	1.00	66.32
VAL107	HG21	1.00	0.104	0.00	0.00
VAL107	H	1.00	1.079	0.00	0.00
THR108	H	0.97	0.000	1.00	-334788.00

3.107.9 Detailed Probabilities of VAL107HG21:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL107	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
V107HA	1.00
V107HG11	1.00
V107HG22	1.00
V107H	1.00
V107HB	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL107	HA	1.00	0.001	1.00	1.18
VAL107	HB	1.00	0.002	1.00	1.24
VAL107	HG11	1.00	0.004	1.00	5.90
VAL107	HG21	1.00	0.001	1.00	51.68
VAL107	H	1.00	0.974	0.00	0.00

3.107.10 Detailed Probabilities of VAL107H:

Overall probability: 0.504

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS106	0.67	1.00
VAL107	0.40	1.00
THR108	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K106HG2	0.98
K106HG3	0.96
K106HA	1.00
K106HB3	1.00
K106HB2	1.00
K106H	1.00
V107HA	1.00
V107HG11	1.00
V107HG21	1.00
V107HB	1.00
V107H	1.00
T108H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS106	HA	1.00	0.008	1.00	0.98
LYS106	HB2	1.00	0.007	1.00	0.23
LYS106	HB3	1.00	0.007	1.00	0.23
LYS106	HG2	0.98	0.029	1.00	0.06
LYS106	HG3	0.96	0.266	0.04	0.00
LYS106	H	1.00	0.134	0.00	0.00
VAL107	HA	1.00	0.051	0.00	0.00
VAL107	HB	1.00	0.046	0.00	0.00
VAL107	HG11	1.00	0.009	1.00	0.61
VAL107	HG21	1.00	0.026	1.00	1.01
VAL107	H	1.00	0.329	0.00	0.00
THR108	H	1.00	0.053	0.00	0.00

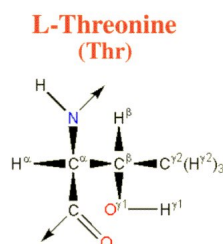
3.108 THR(108)

Figure 107: Image from the BMRB

Residue probability: 0.842

Residue probability confidence: 0.852

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	174.625	174.627	1.788	0.000	0.000
CA 3.108.1	62.221	62.330	4.136	0.471	0.875
CB 3.108.2	69.975	69.395	4.500	1.000	0.833
CG2 3.108.3	21.440	21.588	1.595	1.000	0.800
N 3.108.4	114.072	115.370	5.913	0.900	0.900
HA 3.108.5	4.781	4.461	0.626	0.811	0.875
HB 3.108.6	4.218	4.172	0.855	0.800	0.833
HG2 3.108.7	1.248	1.134	0.349	1.000	0.800
H 3.108.8	8.604	8.272	1.597	0.750	0.900
HG1	NA	—	—	0.000	0.000

3.108.1 Detailed Probabilities of THR108CA:

Overall probability: 0.471

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL107	0.00	1.00
THR108	0.50	0.80
ASP109	0.65	1.00

Expected NOESY Contacts

Proton	Expected probability
V107HA	1.00
T108HB	1.00
T108HG21	1.00
T108H	1.00
T108HG1	1.00
T108HA	1.00
D109HA	1.00
D109H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL107	HA	1.00	0.160	0.00	0.00
THR108	HA	1.00	0.006	1.00	0.19
THR108	HB	1.00	0.557	0.00	0.00
THR108	HG21	1.00	0.023	1.00	0.42
THR108	H	1.00	0.572	0.00	0.00
ASP109	HA	1.00	0.037	0.30	0.00
ASP109	H	1.00	0.004	1.00	0.21

3.108.2 Detailed Probabilities of THR108CB:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
THR108	1.00	0.80
ASP109	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
T108HA	1.00
T108HG21	1.00
T108H	1.00
T108HG1	1.00
T108HB	1.00
D109H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR108	HA	1.00	0.007	1.00	1.20
THR108	HB	1.00	0.004	1.00	9.84
THR108	HG21	1.00	0.001	1.00	2.41
THR108	H	1.00	0.006	1.00	0.45
ASP109	H	1.00	0.002	1.00	0.47

3.108.3 Detailed Probabilities of THR108CG2:

Overall probability: 1.000

Overall confidence: 0.800

Inter- and intra-residue probability

Residue	Probability	Confidence
THR108	1.00	0.80

Expected NOESY Contacts

Proton	Expected probability
T108HA	1.00
T108HB	1.00
T108HG22	1.00
T108H	1.00
T108HG1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR108	HA	1.00	0.003	1.00	1.33
THR108	HB	1.00	0.007	1.00	2.26
THR108	HG21	1.00	0.001	1.00	80.45
THR108	H	1.00	0.009	1.00	0.47

3.108.4 Detailed Probabilities of THR108N:

Overall probability: 0.900

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL107	0.80	1.00
THR108	1.00	0.80
ASP109	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V107HA	1.00
V107H	1.00
V107HG11	0.97
V107HB	1.00
T108HA	1.00
T108HB	1.00
T108HG21	1.00
T108HG1	1.00
T108H	1.00
D109H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL107	HA	1.00	0.005	1.00	-1467072.00
VAL107	HB	1.00	0.002	1.00	-658821.00
VAL107	HG11	0.97	0.000	1.00	-334788.00
VAL107	H	1.00	0.053	0.00	0.00
VAL107	HG21	0.94	0.000	1.00	-714588.00
THR108	HA	1.00	0.004	1.00	-496226.00
THR108	HB	1.00	0.007	1.00	-380706.00
THR108	HG21	1.00	0.000	1.00	-445903.00
THR108	H	1.00	0.004	1.00	-3673402.00
ASP109	H	1.00	0.002	1.00	-1006696.00

3.108.5 Detailed Probabilities of THR108HA:

Overall probability: 0.811

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL107	0.67	1.00
THR108	1.00	0.80
ASP109	0.65	1.00

Expected NOESY Contacts

Proton	Expected probability
V107HA	1.00
T108HB	1.00
T108HG21	1.00
T108H	1.00
T108HG1	1.00
T108HA	1.00
D109HA	1.00
D109H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL107	HA	1.00	0.159	0.00	0.00
VAL107	HB	0.79	0.016	1.00	0.09
VAL107	H	0.91	0.019	1.00	-747524.00
THR108	HA	1.00	0.006	1.00	0.19
THR108	HB	1.00	0.007	1.00	1.20
THR108	HG21	1.00	0.003	1.00	1.33
THR108	H	1.00	0.004	1.00	-496226.00
ASP109	HA	1.00	0.037	0.30	0.00
ASP109	H	1.00	0.021	1.00	-820933.00

3.108.6 Detailed Probabilities of THR108HB:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
THR108	0.75	0.80
ASP109	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
T108HA	1.00
T108HG21	1.00
T108H	1.00
T108HG1	1.00
T108HB	1.00
D109H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR108	HA	1.00	0.557	0.00	0.00
THR108	HB	1.00	0.004	1.00	9.84
THR108	HG21	1.00	0.007	1.00	2.26
THR108	H	1.00	0.007	1.00	-380706.00
ASP109	H	1.00	0.005	1.00	-723223.00

3.108.7 Detailed Probabilities of THR108HG21:

Overall probability: 1.000

Overall confidence: 0.800

Inter- and intra-residue probability

Residue	Probability	Confidence
THR108	1.00	0.80

Expected NOESY Contacts

Proton	Expected probability
T108HA	1.00
T108HB	1.00
T108HG22	1.00
T108H	1.00
T108HG1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR108	HA	1.00	0.023	1.00	0.42
THR108	HB	1.00	0.001	1.00	2.41
THR108	HG21	1.00	0.001	1.00	80.45
THR108	H	1.00	0.000	1.00	-445903.00

3.108.8 Detailed Probabilities of THR108H:

Overall probability: 0.750

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL107	0.60	1.00
THR108	0.75	0.80
ASP109	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V107HA	1.00
V107H	1.00
V107HG11	0.97
V107HB	1.00
T108HA	1.00
T108HB	1.00
T108HG21	1.00
T108HG1	1.00
T108H	1.00
D109H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL107	HA	1.00	0.002	1.00	1.70
VAL107	HB	1.00	0.003	1.00	0.37
VAL107	HG11	0.97	0.040	0.00	0.00
VAL107	H	1.00	0.378	0.00	0.00
VAL107	HG21	0.94	0.023	1.00	1.01
THR108	HA	1.00	0.572	0.00	0.00
THR108	HB	1.00	0.006	1.00	0.45
THR108	HG21	1.00	0.009	1.00	0.47
THR108	H	1.00	0.004	1.00	-3673402.00
ASP109	H	1.00	0.003	1.00	-1568322.00
ASP109	HA	0.84	0.018	1.00	0.28
ASP109	HB2	0.56	0.005	1.00	0.05

3.109 ASP(109)

Figure 108: Image from the BMRB

Residue probability: 0.881

Residue probability confidence: 0.861

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	175.796	176.463	2.348	0.000	0.000
CA 3.109.1	53.849	54.786	4.266	0.775	0.875
CB 3.109.2	43.688	40.949	3.070	1.000	0.833
N 3.109.3	122.574	120.550	5.690	1.000	0.889
HD2	NA	—	—	0.000	0.000
HA 3.109.4	4.738	4.587	0.329	0.900	0.875
HB2 3.109.5	2.816	2.708	0.282	0.800	0.833
HB3 3.109.6	2.729	2.654	0.285	0.800	0.833
H 3.109.7	8.036	8.304	1.027	0.889	0.889

3.109.1 Detailed Probabilities of ASP109CA:

Overall probability: 0.775

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
THR108	0.65	1.00
ASP109	0.73	0.80
ASP110	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
T108HA	1.00
D109HD2	1.00
D109HB2	1.00
D109HB3	1.00
D109H	1.00
D109HA	1.00
D110H	1.00
D110HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR108	HA	1.00	0.037	0.30	0.00
THR108	H	0.84	0.018	1.00	0.28
ASP109	HA	1.00	0.006	1.00	4.38
ASP109	HB2	1.00	0.022	1.00	0.36
ASP109	HB3	1.00	0.031	0.90	0.00
ASP109	H	1.00	0.070	0.00	0.00
ASP110	HA	1.00	0.023	1.00	0.31
ASP110	H	1.00	0.004	1.00	0.83

3.109.2 Detailed Probabilities of ASP109CB:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP109	1.00	0.80
ASP110	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D109HD2	1.00
D109HA	1.00
D109HB3	1.00
D109H	1.00
D109HB2	1.00
D110H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP109	HA	1.00	0.007	1.00	0.78
ASP109	HB2	1.00	0.008	1.00	6.26
ASP109	HB3	1.00	0.000	1.00	4.75
ASP109	H	1.00	0.002	1.00	0.63
ASP110	H	1.00	0.007	1.00	0.36

3.109.3 Detailed Probabilities of ASP109N:

Overall probability: 1.000

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
THR108	1.00	0.75
ASP109	1.00	1.00
ASP110	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
T108HG1	0.98
T108HA	1.00
T108H	1.00
T108HB	1.00
D109HA	1.00
D109HB2	1.00
D109HB3	1.00
D109H	1.00
D110H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR108	HA	1.00	0.021	1.00	-820933.00
THR108	HB	1.00	0.005	1.00	-723223.00
THR108	H	1.00	0.003	1.00	-1568322.00
THR108	HG21	0.94	0.000	1.00	-431201.00
ASP109	HA	1.00	0.022	1.00	-820933.00
ASP109	HB2	1.00	0.004	1.00	-955376.00
ASP109	HB3	1.00	0.002	1.00	-1055396.00
ASP109	H	1.00	0.003	1.00	-8548165.00
ASP110	H	1.00	0.002	1.00	-171345.00

3.109.4 Detailed Probabilities of ASP109HA:

Overall probability: 0.900

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
THR108	0.30	1.00
ASP109	1.00	0.80
ASP110	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
T108HA	1.00
D109HD2	1.00
D109HB2	1.00
D109HB3	1.00
D109H	1.00
D109HA	1.00
D110H	1.00
D110HA	1.00

NOESY contacts detailed probability

3.109 ASP(109)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR108	HA	1.00	0.037	0.30	0.00
ASP109	HA	1.00	0.006	1.00	4.38
ASP109	HB2	1.00	0.007	1.00	0.78
ASP109	HB3	1.00	0.006	1.00	0.70
ASP109	H	1.00	0.022	1.00	-820933.00
ASP110	HA	1.00	0.007	1.00	0.14
ASP110	H	1.00	0.005	1.00	-2635928.00

3.109.5 Detailed Probabilities of ASP109HB2:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP109	0.75	0.80
ASP110	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D109HD2	1.00
D109HA	1.00
D109HB3	1.00
D109H	1.00
D109HB2	1.00
D110H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP109	HA	1.00	0.022	1.00	0.36
ASP109	HB2	1.00	0.008	1.00	6.26
ASP109	HB3	1.00	0.089	0.00	0.00
ASP109	H	1.00	0.004	1.00	-955376.00
ASP110	H	1.00	0.000	1.00	-662804.00

3.109.6 Detailed Probabilities of ASP109HB3:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP109	0.98	0.80
ASP110	0.10	1.00

Expected NOESY Contacts

Proton	Expected probability
D109HD2	1.00
D109HA	1.00
D109HB2	1.00
D109H	1.00
D109HB3	1.00
D110H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP109	HA	1.00	0.031	0.90	0.00
ASP109	HB2	1.00	0.000	1.00	4.75
ASP109	HB3	1.00	0.002	1.00	6.10
ASP109	H	1.00	0.002	1.00	-1055396.00
ASP110	H	1.00	0.039	0.10	0.00

3.109.7 Detailed Probabilities of ASP109H:

Overall probability: 0.889

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
THR108	1.00	0.75
ASP109	0.75	1.00
ASP110	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
T108HG1	0.98
T108HA	1.00
T108H	1.00
T108HB	1.00
D109HA	1.00
D109HB2	1.00
D109HB3	1.00
D109H	1.00
D110H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
THR108	HA	1.00	0.004	1.00	0.21
THR108	HB	1.00	0.002	1.00	0.47
THR108	H	1.00	0.002	1.00	-1006696.00
THR108	HG21	0.94	0.011	1.00	0.20
ASP109	HA	1.00	0.070	0.00	0.00
ASP109	HB2	1.00	0.002	1.00	0.63
ASP109	HB3	1.00	0.006	1.00	0.63
ASP109	H	1.00	0.003	1.00	-8548165.00
ASP110	H	1.00	0.001	1.00	-184460.00

3.110 ASP(110)

Figure 109: Image from the BMRB

Residue probability: 0.707

Residue probability confidence: 0.893

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	177.527	176.463	2.348	0.000	0.000
CA 3.110.1	57.388	54.786	4.266	0.429	0.875
CB 3.110.2	40.301	40.949	3.070	0.833	0.833
N 3.110.3	122.852	120.550	5.690	0.918	1.000
HD2	NA	—	—	0.000	0.000
HA 3.110.4	4.095	4.587	0.329	0.571	0.875
HB2 3.110.5	2.416	2.708	0.282	0.400	0.833
HB3 3.110.6	2.681	2.654	0.285	0.800	0.833
H 3.110.7	8.696	8.304	1.027	1.000	1.000

3.110.1 Detailed Probabilities of ASP110CA:

Overall probability: 0.429

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP109	1.00	1.00
ASP110	0.50	0.80
GLU111	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D109HA	1.00
D110HD2	1.00
D110HB2	1.00
D110HB3	1.00
D110H	1.00
D110HA	1.00
E111H	1.00
E111HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP109	HA	1.00	0.007	1.00	0.14
ASP110	HA	1.00	0.259	0.00	0.00
ASP110	HB2	1.00	0.259	0.00	0.00
ASP110	HB3	1.00	0.006	1.00	0.57
ASP110	H	1.00	0.003	1.00	0.53
GLU111	HA	1.00	0.366	0.00	0.00
GLU111	H	1.00	0.097	0.00	0.00

3.110.2 Detailed Probabilities of ASP110CB:

Overall probability: 0.833

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP110	0.75	0.80
GLU111	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D110HD2	1.00
D110HA	1.00
D110HB3	1.00
D110H	1.00
D110HB2	1.00
E111H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP110	HA	1.00	0.000	1.00	0.67
ASP110	HB2	1.00	0.263	0.00	0.00
ASP110	HB3	1.00	0.002	1.00	2.86
ASP110	H	1.00	0.004	1.00	0.41
GLU111	H	1.00	0.006	1.00	0.34
GLU111	HA	0.54	0.006	1.00	0.10

3.110.3 Detailed Probabilities of ASP110N:

Overall probability: 0.918

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP109	0.77	1.00
ASP110	1.00	1.00
GLU111	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D109HB2	1.00
D109H	1.00
D109HA	1.00
D109HB3	1.00
D110HA	1.00
D110HB2	1.00
D110HB3	1.00
D110H	1.00
E111H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP109	HA	1.00	0.005	1.00	-2635928.00
ASP109	HB2	1.00	0.000	1.00	-662804.00
ASP109	HB3	1.00	0.039	0.10	0.00
ASP109	H	1.00	0.001	1.00	-184460.00
ASP110	HA	1.00	0.000	1.00	-960573.00
ASP110	HB2	1.00	0.001	1.00	-621275.00
ASP110	HB3	1.00	0.009	1.00	-1070928.00
ASP110	H	1.00	0.002	1.00	-8648139.00
GLU111	H	1.00	0.005	1.00	-1052631.00
GLU111	HA	0.86	0.002	1.00	-75438.00
GLU111	HB2	0.58	0.001	1.00	-239552.00

3.110.4 Detailed Probabilities of ASP110HA:

Overall probability: 0.571

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP109	1.00	1.00
ASP110	0.75	0.80
GLU111	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D109HA	1.00
D110HD2	1.00
D110HB2	1.00
D110HB3	1.00
D110H	1.00
D110HA	1.00
E111H	1.00
E111HA	1.00

NOESY contacts detailed probability

3.110 ASP(110)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP109	HA	1.00	0.023	1.00	0.31
ASP110	HA	1.00	0.259	0.00	0.00
ASP110	HB2	1.00	0.000	1.00	0.67
ASP110	HB3	1.00	0.002	1.00	0.64
ASP110	H	1.00	0.000	1.00	-960573.00
GLU111	HA	1.00	0.348	0.00	0.00
GLU111	H	1.00	0.041	0.00	0.00

3.110.5 Detailed Probabilities of ASP110HB2:

Overall probability: 0.400

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP110	0.25	0.80
GLU111	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D110HD2	1.00
D110HA	1.00
D110HB3	1.00
D110H	1.00
D110HB2	1.00
E111H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP110	HA	1.00	0.259	0.00	0.00
ASP110	HB2	1.00	0.263	0.00	0.00
ASP110	HB3	1.00	0.287	0.00	0.00
ASP110	H	1.00	0.001	1.00	-621275.00
GLU111	H	1.00	0.000	1.00	-401129.00

3.110.6 Detailed Probabilities of ASP110HB3:

Overall probability: 0.800

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP110	0.75	0.80
GLU111	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D110HD2	1.00
D110HA	1.00
D110HB2	1.00
D110H	1.00
D110HB3	1.00
E111H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP110	HA	1.00	0.006	1.00	0.57
ASP110	HB2	1.00	0.002	1.00	2.86
ASP110	HB3	1.00	0.164	0.00	0.00
ASP110	H	1.00	0.009	1.00	-1070928.00
GLU111	H	1.00	0.007	1.00	-664166.00

3.110.7 Detailed Probabilities of ASP110H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP109	1.00	1.00
ASP110	1.00	1.00
GLU111	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D109HB2	1.00
D109H	1.00
D109HA	1.00
D109HB3	1.00
D110HA	1.00
D110HB2	1.00
D110HB3	1.00
D110H	1.00
E111H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP109	HA	1.00	0.004	1.00	0.83
ASP109	HB2	1.00	0.007	1.00	0.36
ASP109	HB3	1.00	0.000	1.00	0.30
ASP109	H	1.00	0.002	1.00	-171345.00
ASP110	HA	1.00	0.003	1.00	0.53
ASP110	HB2	1.00	0.004	1.00	0.41
ASP110	HB3	1.00	0.004	1.00	0.49
ASP110	H	1.00	0.002	1.00	-8648139.00
GLU111	H	1.00	0.004	1.00	-766502.00

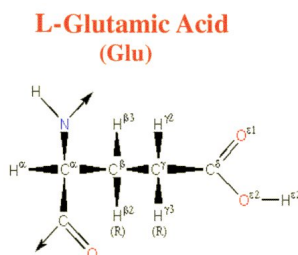


Figure 110: Image from the BMRB

Residue probability: 0.440
Residue probability confidence: 0.925

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	179.942	176.942	2.547	0.000	0.000
CA 3.111.1	59.357	57.442	3.837	0.000	1.000
CB 3.111.2	28.496	30.185	4.018	0.286	0.875
CG 3.111.3	36.010	36.085	1.533	0.714	0.875
N 3.111.4	119.144	120.574	4.837	0.727	1.000
HA 3.111.5	3.988	4.245	0.429	0.364	1.000
HB2 3.111.6	2.099	2.021	0.233	0.571	0.875
HB3 3.111.7	2.023	1.994	0.244	0.000	0.875
HG2 3.111.8	2.287	2.258	0.226	0.503	0.875
HG3 3.111.9	2.269	2.233	0.232	0.505	0.875
H 3.111.10	8.213	8.332	0.601	0.727	1.000
HE2	NA	—	—	0.000	0.000

3.111.1 Detailed Probabilities of GLU111CA:

Overall probability: 0.000
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP110	0.00	1.00
GLU111	0.00	1.00
GLU112	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D110HA	1.00
E111HB2	1.00
E111HB3	1.00
E111HG2	1.00
E111HG3	1.00
E111H	1.00
E111HA	1.00
E112H	1.00
E112HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP110	HA	1.00	0.348	0.00	0.00
GLU111	HA	1.00	0.241	0.00	0.00
GLU111	HB2	1.00	0.086	0.00	0.00
GLU111	HB3	1.00	0.082	0.00	0.00
GLU111	HG2	1.00	0.102	0.00	0.00
GLU111	HG3	1.00	0.084	0.00	0.00
GLU111	H	1.00	0.156	0.00	0.00
GLU112	HA	1.00	0.250	0.00	0.00
GLU112	H	1.00	0.177	0.00	0.00

3.111.2 Detailed Probabilities of GLU111CB:

Overall probability: 0.286

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU111	0.17	0.86
GLU112	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E111HA	1.00
E111HB3	1.00
E111HG2	1.00
E111HG3	1.00
E111H	1.00
E111HE2	1.00
E111HB2	1.00
E112H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU111	HA	1.00	4.239	0.00	0.00
GLU111	HB2	1.00	6.128	0.00	0.00
GLU111	HB3	1.00	6.204	0.00	0.00
GLU111	HG2	1.00	5.940	0.00	0.00
GLU111	HG3	1.00	5.958	0.00	0.00
GLU111	H	1.00	0.014	1.00	1.46
GLU112	H	1.00	0.007	1.00	1.46

3.111.3 Detailed Probabilities of GLU111CG:

Overall probability: 0.714

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU111	0.67	0.86
GLU112	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E111HA	1.00
E111HB2	1.00
E111HB3	1.00
E111HG2	1.00
E111H	1.00
E111HE2	1.00
E111HG3	1.00
E112H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU111	HA	1.00	0.049	0.00	0.00
GLU111	HB2	1.00	0.019	1.00	8.87
GLU111	HB3	1.00	0.057	0.00	0.00
GLU111	HG2	1.00	0.009	1.00	100.68
GLU111	HG3	1.00	0.027	1.00	100.68
GLU111	H	1.00	0.012	1.00	0.66
GLU112	H	0.97	0.009	1.00	0.66

3.111.4 Detailed Probabilities of GLU111N:

Overall probability: 0.727

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP110	0.75	1.00
GLU111	0.67	1.00
GLU112	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
D110H	1.00
D110HA	1.00
D110HB3	1.00
D110HB2	1.00
E111HA	1.00
E111HB2	1.00
E111HB3	1.00
E111HG2	1.00
E111HG3	1.00
E111H	1.00
E112H	1.00

NOESY contacts detailed probability

3.111 GLU(111)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP110	HA	1.00	0.041	0.00	0.00
ASP110	HB2	1.00	0.000	1.00	-401129.00
ASP110	HB3	1.00	0.007	1.00	-664166.00
ASP110	H	1.00	0.004	1.00	-766502.00
GLU111	HA	1.00	0.066	0.00	0.00
GLU111	HB2	1.00	0.030	1.00	-1154493.00
GLU111	HB3	1.00	0.103	0.00	0.00
GLU111	HG2	1.00	0.001	1.00	-993684.00
GLU111	HG3	1.00	0.019	1.00	-993684.00
GLU111	H	1.00	0.005	1.00	-14779317.00
GLU112	H	1.00	0.016	1.00	-14779317.00

3.111.5 Detailed Probabilities of GLU111HA:

Overall probability: 0.364

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP110	0.75	1.00
GLU111	0.00	1.00
GLU112	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
D110HA	1.00
E111HB2	1.00
E111HB3	1.00
E111HG2	1.00
E111HG3	1.00
E111H	1.00
E111HA	1.00
E112H	1.00
E112HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP110	HA	1.00	0.366	0.00	0.00
ASP110	HB2	0.54	0.006	1.00	0.10
ASP110	HB3	0.84	0.002	1.00	0.15
ASP110	H	0.86	0.002	1.00	-75438.00
GLU111	HA	1.00	0.241	0.00	0.00
GLU111	HB2	1.00	4.239	0.00	0.00
GLU111	HG2	1.00	0.049	0.00	0.00
GLU111	HG3	1.00	0.049	0.00	0.00
GLU111	H	1.00	0.066	0.00	0.00
GLU112	HA	1.00	0.054	0.00	0.00
GLU112	H	1.00	0.012	1.00	-1250966.00

3.111.6 Detailed Probabilities of GLU111HB2:

Overall probability: 0.571

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU111	0.60	0.86
GLU112	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E111HA	1.00
E111HB3	1.00
E111HG2	1.00
E111HG3	1.00
E111H	1.00
E111HE2	1.00
E111HB2	1.00
E112H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU111	HA	1.00	0.086	0.00	0.00
GLU111	HB2	1.00	6.128	0.00	0.00
GLU111	HG2	1.00	0.019	1.00	8.87
GLU111	HG3	1.00	0.019	1.00	8.87
GLU111	H	1.00	0.030	1.00	-1154493.00
GLU112	H	1.00	0.252	0.00	0.00
GLU112	HA	0.69	0.021	1.00	5.05

3.111.7 Detailed Probabilities of GLU111HB3:

Overall probability: 0.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU111	0.00	0.86
GLU112	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E111HA	1.00
E111HB2	1.00
E111HG2	1.00
E111HG3	1.00
E111H	1.00
E111HE2	1.00
E111HB3	1.00
E112H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU111	HA	1.00	0.082	0.00	0.00
GLU111	HB2	1.00	6.204	0.00	0.00
GLU111	HG2	1.00	0.057	0.00	0.00
GLU111	HG3	1.00	0.057	0.00	0.00
GLU111	H	1.00	0.103	0.00	0.00
GLU112	H	1.00	0.285	0.00	0.00

3.111.8 Detailed Probabilities of GLU111HG2:

Overall probability: 0.503

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU111	0.60	0.86
GLU112	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
E111HA	1.00
E111HB2	1.00
E111HB3	1.00
E111HG3	1.00
E111H	1.00
E111HE2	1.00
E111HG2	1.00
E112H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU111	HA	1.00	0.102	0.00	0.00
GLU111	HB2	1.00	5.940	0.00	0.00
GLU111	HG2	1.00	0.009	1.00	100.68
GLU111	HG3	1.00	0.009	1.00	100.68
GLU111	H	1.00	0.001	1.00	-993684.00
GLU112	H	0.98	0.064	0.02	0.00

3.111.9 Detailed Probabilities of GLU111HG3:

Overall probability: 0.505

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU111	0.60	0.86
GLU112	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
E111HA	1.00
E111HB2	1.00
E111HB3	1.00
E111HG2	1.00
E111H	1.00
E111HE2	1.00
E111HG3	1.00
E112H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU111	HA	1.00	0.084	0.00	0.00
GLU111	HB2	1.00	5.958	0.00	0.00
GLU111	HG2	1.00	0.027	1.00	100.68
GLU111	HG3	1.00	0.027	1.00	100.68
GLU111	H	1.00	0.019	1.00	-993684.00
GLU112	H	0.97	0.082	0.03	0.00

3.111.10 Detailed Probabilities of GLU111H:

Overall probability: 0.727

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ASP110	0.75	1.00
GLU111	0.80	1.00
GLU112	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
D110H	1.00
D110HA	1.00
D110HB3	1.00
D110HB2	1.00
E111HA	1.00
E111HB2	1.00
E111HB3	1.00
E111HG2	1.00
E111HG3	1.00
E111H	1.00
E112H	1.00

NOESY contacts detailed probability

3.111 GLU(111)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ASP110	HA	1.00	0.097	0.00	0.00
ASP110	HB2	1.00	0.006	1.00	0.34
ASP110	HB3	1.00	0.006	1.00	0.46
ASP110	H	1.00	0.005	1.00	-1052631.00
GLU111	HA	1.00	0.156	0.00	0.00
GLU111	HB2	1.00	0.014	1.00	1.46
GLU111	HG2	1.00	0.016	1.00	1.06
GLU111	HG3	1.00	0.012	1.00	0.66
GLU111	H	1.00	0.005	1.00	-14779317.00
GLU112	H	1.00	0.170	0.00	0.00
GLU112	HB2	0.67	0.014	1.00	1.46

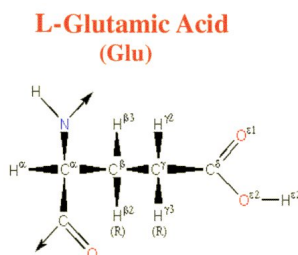


Figure 111: Image from the BMRB

Residue probability: 0.629
Residue probability confidence: 0.925

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.430	176.942	2.547	0.000	0.000
CA 3.112.1	58.749	57.442	3.837	0.400	1.000
CB 3.112.2	29.194	30.185	4.018	0.888	0.875
CG 3.112.3	36.010	36.085	1.533	0.586	0.875
N 3.112.4	121.400	120.574	4.837	0.360	1.000
HA 3.112.5	3.997	4.245	0.429	0.378	1.000
HB2 3.112.6	2.084	2.021	0.233	0.875	0.875
HB3 3.112.7	2.083	1.994	0.244	0.875	0.875
HG2 3.112.8	2.337	2.258	0.226	0.571	0.875
HG3 3.112.9	2.338	2.233	0.232	0.571	0.875
H 3.112.10	8.234	8.332	0.601	0.786	1.000
HE2	NA	—	—	0.000	0.000

3.112.1 Detailed Probabilities of GLU112CA:

Overall probability: 0.400
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU111	0.50	1.00
GLU112	0.33	1.00
ALA113	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E111HA	1.00
E112HB2	1.00
E112HB3	1.00
E112HG2	1.00
E112HG3	1.00
E112H	1.00
E112HA	1.00
A113HA	1.00
A113H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU111	HA	1.00	0.054	0.00	0.00
GLU111	HB2	0.69	0.021	1.00	5.05
GLU112	HA	1.00	0.045	0.00	0.00
GLU112	HB2	1.00	0.006	1.00	5.05
GLU112	HB3	1.00	0.005	1.00	5.05
GLU112	HG2	1.00	0.259	0.00	0.00
GLU112	HG3	1.00	0.260	0.00	0.00
GLU112	H	1.00	0.045	0.00	0.00
ALA113	HA	1.00	0.242	0.00	0.00
ALA113	H	1.00	0.026	1.00	1.04

3.112.2 Detailed Probabilities of GLU112CB:

Overall probability: 0.888

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU112	0.85	0.86
ALA113	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E112HA	1.00
E112HB3	1.00
E112HG2	1.00
E112HG3	1.00
E112H	1.00
E112HE2	1.00
E112HB2	1.00
A113H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU112	HA	1.00	0.039	0.10	0.00
GLU112	HB2	1.00	0.009	1.00	35.26
GLU112	HB3	1.00	0.010	1.00	35.26
GLU112	HG2	1.00	0.002	1.00	4.32
GLU112	HG3	1.00	0.003	1.00	4.32
GLU112	H	1.00	0.007	1.00	1.46
ALA113	H	1.00	0.015	1.00	1.50
ALA113	HA	0.83	0.000	1.00	0.19

3.112.3 Detailed Probabilities of GLU112CG:

Overall probability: 0.586

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU112	0.52	0.86
ALA113	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E112HA	1.00
E112HB2	1.00
E112HB3	1.00
E112HG3	1.00
E112H	1.00
E112HE2	1.00
E112HG2	1.00
A113H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU112	HA	1.00	0.039	0.10	0.00
GLU112	HB2	1.00	0.004	1.00	8.87
GLU112	HB3	1.00	0.003	1.00	8.87
GLU112	HG2	1.00	0.381	0.00	0.00
GLU112	HG3	1.00	0.380	0.00	0.00
GLU112	H	1.00	0.005	1.00	1.06
ALA113	H	0.97	0.021	1.00	0.69

3.112.4 Detailed Probabilities of GLU112N:

Overall probability: 0.360

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU111	0.17	1.00
GLU112	0.50	1.00
ALA113	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E111HG2	0.98
E111HA	1.00
E111H	1.00
E111HB3	1.00
E111HG3	0.97
E111HB2	1.00
E112HA	1.00
E112HB2	1.00
E112HB3	1.00
E112HG2	1.00
E112HG3	1.00
E112H	1.00
A113H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU111	HA	1.00	0.012	1.00	-1250966.00
GLU111	HB2	1.00	0.252	0.00	0.00
GLU111	HB3	1.00	0.285	0.00	0.00
GLU111	HG2	0.98	0.064	0.02	0.00
GLU111	HG3	0.97	0.082	0.03	0.00
GLU111	H	1.00	0.170	0.00	0.00
GLU112	HA	1.00	0.003	1.00	-1250966.00
GLU112	HB2	1.00	0.267	0.00	0.00
GLU112	HB3	1.00	0.268	0.00	0.00
GLU112	HG2	1.00	0.014	1.00	-594594.00
GLU112	HG3	1.00	0.013	1.00	-594594.00
GLU112	H	1.00	0.149	0.00	0.00
ALA113	H	1.00	0.265	0.00	0.00
ALA113	HB1	0.52	0.004	1.00	-285643.00

3.112.5 Detailed Probabilities of GLU112HA:

Overall probability: 0.378

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU111	0.00	1.00
GLU112	0.23	1.00
ALA113	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E111HA	1.00
E112HB2	1.00
E112HB3	1.00
E112HG2	1.00
E112HG3	1.00
E112H	1.00
E112HA	1.00
A113HA	1.00
A113H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU111	HA	1.00	0.250	0.00	0.00
GLU112	HA	1.00	0.045	0.00	0.00
GLU112	HB2	1.00	0.039	0.10	0.00
GLU112	HB3	1.00	0.039	0.10	0.00
GLU112	HG2	1.00	0.039	0.10	0.00
GLU112	HG3	1.00	0.039	0.10	0.00
GLU112	H	1.00	0.003	1.00	-1250966.00
ALA113	HA	1.00	0.027	1.00	0.06
ALA113	H	1.00	0.005	1.00	-457960.00

3.112.6 Detailed Probabilities of GLU112HB2:

Overall probability: 0.875

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU112	0.83	0.86
ALA113	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E112HA	1.00
E112HB3	1.00
E112HG2	1.00
E112HG3	1.00
E112H	1.00
E112HE2	1.00
E112HB2	1.00
A113H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU112	HA	1.00	0.005	1.00	5.05
GLU112	HB2	1.00	0.010	1.00	35.26
GLU112	HB3	1.00	0.010	1.00	35.26
GLU112	HG2	1.00	0.003	1.00	8.87
GLU112	HG3	1.00	0.003	1.00	8.87
GLU112	H	1.00	0.267	0.00	0.00
ALA113	H	1.00	0.028	1.00	-2103946.00
ALA113	HA	0.83	0.017	1.00	0.17

3.112.7 Detailed Probabilities of GLU112HB3:

Overall probability: 0.875

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU112	0.83	0.86
ALA113	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E112HA	1.00
E112HB2	1.00
E112HG2	1.00
E112HG3	1.00
E112H	1.00
E112HE2	1.00
E112HB3	1.00
A113H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU112	HA	1.00	0.005	1.00	5.05
GLU112	HB2	1.00	0.010	1.00	35.26
GLU112	HB3	1.00	0.010	1.00	35.26
GLU112	HG2	1.00	0.003	1.00	8.87
GLU112	HG3	1.00	0.003	1.00	8.87
GLU112	H	1.00	0.267	0.00	0.00
ALA113	H	1.00	0.028	1.00	-2103946.00
ALA113	HA	0.83	0.017	1.00	0.17

3.112.8 Detailed Probabilities of GLU112HG2:

Overall probability: 0.571

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU112	0.50	0.86
ALA113	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E112HA	1.00
E112HB2	1.00
E112HB3	1.00
E112HG3	1.00
E112H	1.00
E112HE2	1.00
E112HG2	1.00
A113H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU112	HA	1.00	0.259	0.00	0.00
GLU112	HB2	1.00	0.003	1.00	4.32
GLU112	HB3	1.00	0.003	1.00	4.32
GLU112	HG2	1.00	0.380	0.00	0.00
GLU112	HG3	1.00	0.381	0.00	0.00
GLU112	H	1.00	0.013	1.00	-594594.00
ALA113	H	0.97	0.017	1.00	-161138.00

3.112.9 Detailed Probabilities of GLU112HG3:

Overall probability: 0.571

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU112	0.50	0.86
ALA113	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E112HA	1.00
E112HB2	1.00
E112HB3	1.00
E112HG2	1.00
E112H	1.00
E112HE2	1.00
E112HG3	1.00
A113H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU112	HA	1.00	0.259	0.00	0.00
GLU112	HB2	1.00	0.003	1.00	4.32
GLU112	HB3	1.00	0.003	1.00	4.32
GLU112	HG2	1.00	0.380	0.00	0.00
GLU112	HG3	1.00	0.381	0.00	0.00
GLU112	H	1.00	0.013	1.00	-594594.00
ALA113	H	0.97	0.017	1.00	-161138.00

3.112.10 Detailed Probabilities of GLU112H:

Overall probability: 0.786

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU111	0.80	1.00
GLU112	0.67	1.00
ALA113	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E111HG2	0.98
E111HA	1.00
E111H	1.00
E111HB3	1.00
E111HG3	0.97
E111HB2	1.00
E112HA	1.00
E112HB2	1.00
E112HB3	1.00
E112HG2	1.00
E112HG3	1.00
E112H	1.00
A113H	1.00

NOESY contacts detailed probability

3.112 GLU(112)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU111	HA	1.00	0.177	0.00	0.00
GLU111	HB2	1.00	0.007	1.00	1.46
GLU111	HG2	0.98	0.005	1.00	1.06
GLU111	HG3	0.97	0.009	1.00	0.66
GLU111	H	1.00	0.016	1.00	-14779317.00
GLU112	HA	1.00	0.045	0.00	0.00
GLU112	HB2	1.00	0.007	1.00	1.46
GLU112	HB3	1.00	0.007	1.00	1.46
GLU112	HG2	1.00	0.005	1.00	1.06
GLU112	HG3	1.00	0.005	1.00	1.06
GLU112	H	1.00	0.149	0.00	0.00
ALA113	H	1.00	0.003	1.00	-1317750.00
ALA113	HA	0.90	0.001	1.00	0.06
ALA113	HB1	0.52	0.003	1.00	0.23

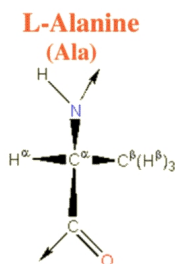


Figure 112: Image from the BMRB

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
CA 3.113.1	55.382	53.289	3.425	0.889	1.000
CB 3.113.2	18.602	19.355	4.103	1.000	1.000
N 3.113.3	120.316	123.100	4.487	1.000	1.000
HA 3.113.4	3.800	4.254	0.459	0.750	1.000
HB 3.113.5	1.410	1.346	0.258	1.000	1.000
H 3.113.6	8.118	8.206	0.601	0.917	1.000

3.113.1 Detailed Probabilities of ALA113CA:

Overall probability: 0.889
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU112	1.00	1.00
ALA113	1.00	1.00
LEU114	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E112HA	1.00
A113H	1.00
A113HB1	1.00
A113HA	1.00
L114H	1.00
L114HA	1.00

NOESY contacts detailed probability

3.113 ALA(113)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU112	HA	1.00	0.027	1.00	0.06
GLU112	HB2	0.70	0.016	1.00	0.17
GLU112	HB3	0.83	0.017	1.00	0.17
GLU112	H	0.90	0.001	1.00	0.06
ALA113	HA	1.00	0.003	1.00	3.95
ALA113	HB1	1.00	0.003	1.00	1.28
ALA113	H	1.00	0.000	1.00	0.49
LEU114	HA	1.00	0.090	0.00	0.00
LEU114	H	1.00	0.008	1.00	0.11

3.113.2 Detailed Probabilities of ALA113CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ALA113	1.00	1.00
LEU114	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
A113HA	1.00
A113H	1.00
A113HB2	1.00
L114H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA113	HA	1.00	0.001	1.00	1.74
ALA113	HB1	1.00	0.003	1.00	34.53
ALA113	H	1.00	0.001	1.00	1.79
LEU114	H	1.00	0.006	1.00	0.90

3.113.3 Detailed Probabilities of ALA113N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU112	1.00	1.00
ALA113	1.00	1.00
LEU114	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E112HB2	1.00
E112HG3	0.97
E112HA	1.00
E112H	1.00
E112HG2	0.98
E112HB3	1.00
A113HA	1.00
A113HB1	1.00
A113H	1.00
L114H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU112	HA	1.00	0.005	1.00	-457960.00
GLU112	HB2	1.00	0.029	1.00	-2103946.00
GLU112	HB3	1.00	0.028	1.00	-2103946.00
GLU112	HG2	0.98	0.018	1.00	-161138.00
GLU112	HG3	0.97	0.017	1.00	-161138.00
GLU112	H	1.00	0.003	1.00	-1317750.00
ALA113	HA	1.00	0.001	1.00	-931615.00
ALA113	HB1	1.00	0.002	1.00	-2727490.00
ALA113	H	1.00	0.005	1.00	-16420475.00
LEU114	H	1.00	0.004	1.00	-824704.00
LEU114	HA	0.92	0.009	1.00	-448057.00
LEU114	HB2	0.71	0.003	1.00	-292311.00

3.113.4 Detailed Probabilities of ALA113HA:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU112	0.67	1.00
ALA113	1.00	1.00
LEU114	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
E112HA	1.00
A113H	1.00
A113HB1	1.00
A113HA	1.00
L114H	1.00
L114HA	1.00

NOESY contacts detailed probability

3.113 ALA(113)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU112	HA	1.00	0.242	0.00	0.00
GLU112	HB2	0.70	0.000	1.00	0.19
GLU112	HB3	0.83	0.000	1.00	0.19
ALA113	HA	1.00	0.003	1.00	3.95
ALA113	HB1	1.00	0.001	1.00	1.74
ALA113	H	1.00	0.001	1.00	-931615.00
LEU114	HA	1.00	0.091	0.00	0.00
LEU114	H	1.00	0.003	1.00	-251903.00

3.113.5 Detailed Probabilities of ALA113HB1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ALA113	1.00	1.00
LEU114	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
A113HA	1.00
A113H	1.00
A113HB2	1.00
L114H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA113	HA	1.00	0.003	1.00	1.28
ALA113	HB1	1.00	0.003	1.00	34.53
ALA113	H	1.00	0.002	1.00	-2727490.00
LEU114	H	1.00	0.003	1.00	-1927322.00
LEU114	HA	0.71	0.006	1.00	0.60

3.113.6 Detailed Probabilities of ALA113H:

Overall probability: 0.917

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU112	0.83	1.00
ALA113	1.00	1.00
LEU114	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E112HB2	1.00
E112HG3	0.97
E112HA	1.00
E112H	1.00
E112HG2	0.98
E112HB3	1.00
A113HA	1.00
A113HB1	1.00
A113H	1.00
L114H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU112	HA	1.00	0.026	1.00	1.04
GLU112	HB2	1.00	0.015	1.00	1.50
GLU112	HB3	1.00	0.015	1.00	1.50
GLU112	HG2	0.98	0.021	1.00	0.69
GLU112	HG3	0.97	0.021	1.00	0.69
GLU112	H	1.00	0.265	0.00	0.00
ALA113	HA	1.00	0.000	1.00	0.49
ALA113	HB1	1.00	0.001	1.00	1.79
ALA113	H	1.00	0.005	1.00	-16420475.00
LEU114	H	1.00	0.000	1.00	-878205.00
LEU114	HA	0.92	0.013	1.00	0.31
LEU114	HB2	0.71	0.003	1.00	0.07

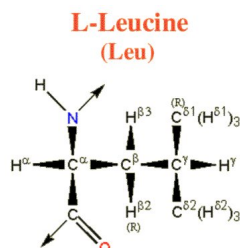


Figure 113: Image from the BMRB

Residue probability: 0.874
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.431	177.056	1.929	0.000	0.000
CA 3.114.1	57.675	55.735	3.802	0.750	1.000
CB 3.114.2	40.936	42.389	3.750	1.000	1.000
CG 3.114.3	26.770	26.892	3.086	0.752	1.000
CD1 3.114.4	24.730	24.837	3.657	0.857	1.000
CD2 3.114.5	23.240	24.201	3.117	1.000	1.000
N 3.114.6	116.901	121.785	4.943	1.000	1.000
HA 3.114.7	3.713	4.315	0.840	0.818	1.000
HB2 3.114.8	1.735	1.601	0.373	1.000	1.000
HB3 3.114.9	1.397	1.508	0.398	1.000	1.000
HG 3.114.10	1.651	1.510	0.340	0.752	1.000
HD1 3.114.11	0.805	0.739	0.294	0.857	1.000
HD2 3.114.12	0.670	0.727	0.421	0.571	1.000
H 3.114.13	7.743	8.237	0.647	1.000	1.000

3.114.1 Detailed Probabilities of LEU114CA:

Overall probability: 0.750
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ALA113	0.67	1.00
LEU114	0.86	1.00
LYS115	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
A113HA	1.00
L114HB2	1.00
L114HB3	1.00
L114HG	1.00
L114HD11	0.99
L114HD21	0.99
L114H	1.00
L114HA	1.00
K115HA	1.00
K115H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA113	HA	1.00	0.091	0.00	0.00
ALA113	HB1	0.69	0.006	1.00	0.60
ALA113	H	0.92	0.013	1.00	0.31
LEU114	HA	1.00	0.004	1.00	4.57
LEU114	HB2	1.00	0.005	1.00	0.47
LEU114	HB3	1.00	0.007	1.00	0.60
LEU114	HG	1.00	0.079	0.00	0.00
LEU114	HD11	0.99	0.021	1.00	0.43
LEU114	HD21	0.99	0.006	1.00	1.11
LEU114	H	1.00	0.005	1.00	0.42
LYS115	HA	1.00	0.091	0.00	0.00
LYS115	H	1.00	0.011	1.00	0.18

3.114.2 Detailed Probabilities of LEU114CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU114	1.00	1.00
LYS115	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L114HA	1.00
L114HB3	1.00
L114HG	1.00
L114HD11	1.00
L114HD21	1.00
L114H	1.00
L114HB2	1.00
K115H	1.00

NOESY contacts detailed probability

3.114 LEU(114)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU114	HA	1.00	0.003	1.00	0.53
LEU114	HB2	1.00	0.004	1.00	4.26
LEU114	HB3	1.00	0.006	1.00	3.70
LEU114	HG	1.00	0.023	1.00	0.93
LEU114	HD11	1.00	0.006	1.00	0.81
LEU114	HD21	1.00	0.007	1.00	0.60
LEU114	H	1.00	0.004	1.00	0.70
LYS115	H	1.00	0.018	1.00	0.53
LYS115	HA	0.70	0.013	1.00	0.65

3.114.3 Detailed Probabilities of LEU114CG:

Overall probability: 0.752

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU114	0.86	1.00
LYS115	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
L114HA	1.00
L114HB2	1.00
L114HB3	1.00
L114HD11	1.00
L114HD21	1.00
L114H	1.00
L114HG	1.00
K115H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU114	HA	1.00	0.007	1.00	0.40
LEU114	HB2	1.00	0.030	1.00	2.53
LEU114	HB3	1.00	0.027	1.00	0.91
LEU114	HG	1.00	0.015	1.00	19.97
LEU114	HD11	1.00	0.009	1.00	2.48
LEU114	HD21	1.00	0.042	0.00	0.00
LEU114	H	1.00	0.009	1.00	0.63
LYS115	H	0.98	0.135	0.02	0.00

3.114.4 Detailed Probabilities of LEU114CD1:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU114	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
L114HA	0.99
L114HB2	1.00
L114HB3	1.00
L114HG	1.00
L114HD12	1.00
L114HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU114	HA	0.99	0.015	1.00	0.84
LEU114	HB2	1.00	0.007	1.00	2.62
LEU114	HB3	1.00	0.026	1.00	3.41
LEU114	HG	1.00	0.008	1.00	4.39
LEU114	HD11	1.00	0.011	1.00	196.23
LEU114	HD21	1.00	0.461	0.00	0.00
LEU114	H	0.86	0.006	1.00	0.19

3.114.5 Detailed Probabilities of LEU114CD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU114	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L114HA	0.99
L114HB2	1.00
L114HB3	1.00
L114HG	1.00
L114HD11	1.00
L114HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU114	HA	0.99	0.004	1.00	1.65
LEU114	HB2	1.00	0.006	1.00	1.24
LEU114	HB3	1.00	0.007	1.00	1.36
LEU114	HG	1.00	0.006	1.00	1.97
LEU114	HD11	1.00	0.001	1.00	4.28
LEU114	HD21	1.00	0.003	1.00	77.31
LEU114	H	0.85	0.003	1.00	0.37

3.114.6 Detailed Probabilities of LEU114N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ALA113	1.00	1.00
LEU114	1.00	1.00
LYS115	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
A113HB1	1.00
A113HA	1.00
A113H	1.00
L114HA	1.00
L114HB2	1.00
L114HB3	1.00
L114HG	1.00
L114H	1.00
K115H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA113	HA	1.00	0.003	1.00	-251903.00
ALA113	HB1	1.00	0.003	1.00	-1927322.00
ALA113	H	1.00	0.000	1.00	-878205.00
LEU114	HA	1.00	0.006	1.00	-685772.00
LEU114	HB2	1.00	0.005	1.00	-1095726.00
LEU114	HB3	1.00	0.010	1.00	-1927322.00
LEU114	HG	1.00	0.005	1.00	-1140525.00
LEU114	H	1.00	0.005	1.00	-7419162.00
LEU114	HD11	0.88	0.015	1.00	-523224.00
LEU114	HD21	0.87	0.003	1.00	-519533.00
LYS115	H	1.00	0.002	1.00	-808297.00
LYS115	HA	0.89	0.003	1.00	-251903.00
LYS115	HB2	0.58	0.001	1.00	-130741.00

3.114.7 Detailed Probabilities of LEU114HA:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ALA113	0.50	1.00
LEU114	1.00	1.00
LYS115	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
A113HA	1.00
L114HB2	1.00
L114HB3	1.00
L114HG	1.00
L114HD11	0.99
L114HD21	0.99
L114H	1.00
L114HA	1.00
K115HA	1.00
K115H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA113	HA	1.00	0.090	0.00	0.00
ALA113	H	0.92	0.009	1.00	-448057.00
LEU114	HA	1.00	0.004	1.00	4.57
LEU114	HB2	1.00	0.003	1.00	0.53
LEU114	HB3	1.00	0.002	1.00	0.62
LEU114	HG	1.00	0.007	1.00	0.40
LEU114	HD11	0.99	0.015	1.00	0.84
LEU114	HD21	0.99	0.004	1.00	1.65
LEU114	H	1.00	0.006	1.00	-685772.00
LYS115	HA	1.00	0.087	0.00	0.00
LYS115	H	1.00	0.001	1.00	-298211.00

3.114.8 Detailed Probabilities of LEU114HB2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU114	1.00	1.00
LYS115	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L114HA	1.00
L114HB3	1.00
L114HG	1.00
L114HD11	1.00
L114HD21	1.00
L114H	1.00
L114HB2	1.00
K115H	1.00

NOESY contacts detailed probability

3.114 LEU(114)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU114	HA	1.00	0.005	1.00	0.47
LEU114	HB2	1.00	0.004	1.00	4.26
LEU114	HB3	1.00	0.004	1.00	3.76
LEU114	HG	1.00	0.030	1.00	2.53
LEU114	HD11	1.00	0.007	1.00	2.62
LEU114	HD21	1.00	0.006	1.00	1.24
LEU114	H	1.00	0.005	1.00	-1095726.00
LYS115	H	1.00	0.011	1.00	-509652.00

3.114.9 Detailed Probabilities of LEU114HB3:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU114	1.00	1.00
LYS115	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L114HA	1.00
L114HB2	1.00
L114HG	1.00
L114HD11	1.00
L114HD21	1.00
L114H	1.00
L114HB3	1.00
K115H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU114	HA	1.00	0.007	1.00	0.60
LEU114	HB2	1.00	0.006	1.00	3.70
LEU114	HB3	1.00	0.002	1.00	5.42
LEU114	HG	1.00	0.027	1.00	0.91
LEU114	HD11	1.00	0.026	1.00	3.41
LEU114	HD21	1.00	0.007	1.00	1.36
LEU114	H	1.00	0.010	1.00	-1927322.00
LYS115	H	1.00	0.014	1.00	-388179.00

3.114.10 Detailed Probabilities of LEU114HG:

Overall probability: 0.752

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU114	0.86	1.00
LYS115	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
L114HA	1.00
L114HB2	1.00
L114HB3	1.00
L114HD11	1.00
L114HD21	1.00
L114H	1.00
L114HG	1.00
K115H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU114	HA	1.00	0.079	0.00	0.00
LEU114	HB2	1.00	0.023	1.00	0.93
LEU114	HB3	1.00	0.019	1.00	1.02
LEU114	HG	1.00	0.015	1.00	19.97
LEU114	HD11	1.00	0.008	1.00	4.39
LEU114	HD21	1.00	0.006	1.00	1.97
LEU114	H	1.00	0.005	1.00	-1140525.00
LYS115	H	0.98	0.095	0.02	0.00

3.114.11 Detailed Probabilities of LEU114HD11:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU114	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
L114HA	0.99
L114HB2	1.00
L114HB3	1.00
L114HG	1.00
L114HD12	1.00
L114HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU114	HA	0.99	0.021	1.00	0.43
LEU114	HB2	1.00	0.006	1.00	0.81
LEU114	HB3	1.00	0.079	0.00	0.00
LEU114	HG	1.00	0.009	1.00	2.48
LEU114	HD11	1.00	0.011	1.00	196.23
LEU114	HD21	1.00	0.001	1.00	4.28
LEU114	H	0.86	0.015	1.00	-523224.00

3.114.12 Detailed Probabilities of LEU114HD21:

Overall probability: 0.571

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU114	0.57	1.00

Expected NOESY Contacts

Proton	Expected probability
L114HA	0.99
L114HB2	1.00
L114HB3	1.00
L114HG	1.00
L114HD11	1.00
L114HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU114	HA	0.99	0.006	1.00	1.11
LEU114	HB2	1.00	0.007	1.00	0.60
LEU114	HB3	1.00	0.056	0.00	0.00
LEU114	HG	1.00	0.042	0.00	0.00
LEU114	HD11	1.00	0.461	0.00	0.00
LEU114	HD21	1.00	0.003	1.00	77.31
LEU114	H	0.85	0.003	1.00	-519533.00

3.114.13 Detailed Probabilities of LEU114H:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ALA113	1.00	1.00
LEU114	1.00	1.00
LYS115	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
A113HB1	1.00
A113HA	1.00
A113H	1.00
L114HA	1.00
L114HB2	1.00
L114HB3	1.00
L114HG	1.00
L114H	1.00
K115H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA113	HA	1.00	0.008	1.00	0.11
ALA113	HB1	1.00	0.006	1.00	0.90
ALA113	H	1.00	0.004	1.00	-824704.00
LEU114	HA	1.00	0.005	1.00	0.42
LEU114	HB2	1.00	0.004	1.00	0.70
LEU114	HB3	1.00	0.002	1.00	0.54
LEU114	HG	1.00	0.009	1.00	0.63
LEU114	H	1.00	0.005	1.00	-7419162.00
LEU114	HD11	0.88	0.006	1.00	0.19
LEU114	HD21	0.87	0.003	1.00	0.37
LYS115	H	1.00	0.005	1.00	-990666.00
LYS115	HA	0.89	0.004	1.00	0.10



Figure 114: Image from the BMRB

Residue probability: 0.820
Residue probability confidence: 0.943

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	179.404	176.660	3.133	0.000	0.000
CA 3.115.1	59.883	57.014	3.028	0.420	1.000
CB 3.115.2	32.178	32.981	3.186	0.900	1.000
CG 3.115.3	24.910	24.941	1.956	0.904	0.909
CD 3.115.4	29.549	29.020	2.193	0.778	0.889
CE 3.115.5	41.780	41.893	1.492	1.000	0.875
N 3.115.6	119.066	120.954	4.210	0.916	1.000
NZ	NA	—	—	0.000	0.000
HA 3.115.7	3.800	4.262	0.489	0.929	1.000
HB2 3.115.8	1.928	1.774	0.365	0.909	1.000
HB3 3.115.9	1.934	1.742	0.385	0.891	1.000
HG2 3.115.10	1.561	1.358	0.344	0.703	0.909
HG3 3.115.11	1.300	1.343	0.357	0.500	0.909
HD2 3.115.12	1.656	1.614	0.957	0.752	0.889
HD3 3.115.13	1.659	1.595	0.387	0.753	0.889
HE 3.115.14	2.909	2.907	0.230	1.000	0.875
H 3.115.15	7.617	8.185	0.605	0.939	1.000
HZ	NA	—	—	0.000	0.000

3.115.1 Detailed Probabilities of LYS115CA:

Overall probability: 0.420
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU114	0.50	1.00
LYS115	0.38	1.00
ILE116	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
L114HA	1.00
K115HB2	1.00
K115HB3	1.00
K115HG2	1.00
K115HG3	1.00
K115HD2	0.98
K115HD3	0.98
K115H	1.00
K115HA	1.00
I116HA	1.00
I116H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU114	HA	1.00	0.087	0.00	0.00
LEU114	H	0.89	0.004	1.00	0.10
LYS115	HA	1.00	0.000	1.00	13.14
LYS115	HB2	1.00	0.370	0.00	0.00
LYS115	HB3	1.00	0.376	0.00	0.00
LYS115	HG2	1.00	0.003	1.00	0.96
LYS115	HG3	1.00	0.222	0.00	0.00
LYS115	HD2	0.98	0.098	0.02	0.00
LYS115	HD3	0.98	0.101	0.02	0.00
LYS115	H	1.00	0.009	1.00	0.97
ILE116	HA	1.00	0.304	0.00	0.00
ILE116	H	1.00	0.027	1.00	0.77

3.115.2 Detailed Probabilities of LYS115CB:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS115	0.89	1.00
ILE116	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K115HA	1.00
K115HB2	1.00
K115HG2	1.00
K115HG3	1.00
K115HD2	1.00
K115HD3	1.00
K115HE2	0.99
K115H	1.00
K115HB3	1.00
I116H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS115	HA	1.00	0.021	1.00	2.44
LYS115	HB2	1.00	0.024	1.00	53.87
LYS115	HB3	1.00	0.030	1.00	0.00
LYS115	HG2	1.00	0.022	1.00	3.20
LYS115	HG3	1.00	0.283	0.00	0.00
LYS115	HD2	1.00	0.027	1.00	5.56
LYS115	HD3	1.00	0.024	1.00	5.56
LYS115	HE2	0.99	0.020	1.00	0.70
LYS115	H	1.00	0.002	1.00	2.14
ILE116	H	1.00	0.027	1.00	1.13

3.115.3 Detailed Probabilities of LYS115CG:

Overall probability: 0.904

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS115	1.00	0.90
ILE116	0.04	1.00

Expected NOESY Contacts

Proton	Expected probability
K115HA	1.00
K115HB2	1.00
K115HB3	1.00
K115HG2	1.00
K115HD2	1.00
K115HD3	1.00
K115HE2	1.00
K115H	1.00
K115HZ2	1.00
K115HG3	1.00
I116H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS115	HA	1.00	0.004	1.00	0.46
LYS115	HB2	1.00	0.013	1.00	1.00
LYS115	HB3	1.00	0.007	1.00	1.00
LYS115	HG2	1.00	0.003	1.00	5.34
LYS115	HG3	1.00	0.002	1.00	15.45
LYS115	HD2	1.00	0.002	1.00	2.37
LYS115	HD3	1.00	0.005	1.00	2.37
LYS115	HE2	1.00	0.005	1.00	0.63
LYS115	H	1.00	0.004	1.00	0.28
ILE116	H	0.96	0.173	0.04	0.00

3.115.4 Detailed Probabilities of LYS115CD:

Overall probability: 0.778

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS115	0.78	0.89

Expected NOESY Contacts

Proton	Expected probability
K115HA	0.98
K115HB2	1.00
K115HB3	1.00
K115HG2	1.00
K115HG3	1.00
K115HD3	1.00
K115HE2	1.00
K115HZ2	1.00
K115HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS115	HA	0.98	0.009	1.00	0.59
LYS115	HB2	1.00	0.004	1.00	5.45
LYS115	HB3	1.00	0.002	1.00	5.45
LYS115	HG2	1.00	0.158	0.00	0.00
LYS115	HG3	1.00	0.103	0.00	0.00
LYS115	HD2	1.00	0.028	1.00	244.35
LYS115	HD3	1.00	0.025	1.00	244.35
LYS115	HE2	1.00	0.004	1.00	4.26
LYS115	H	0.88	0.002	1.00	0.43

3.115.5 Detailed Probabilities of LYS115CE:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS115	1.00	0.88

Expected NOESY Contacts

Proton	Expected probability
K115HB2	0.98
K115HB3	0.99
K115HG2	1.00
K115HG3	1.00
K115HD2	1.00
K115HD3	1.00
K115HE3	1.00
K115HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS115	HB2	0.99	0.013	1.00	1.28
LYS115	HB3	0.99	0.019	1.00	1.28
LYS115	HG2	1.00	0.001	1.00	1.96
LYS115	HG3	1.00	0.009	1.00	0.77
LYS115	HD2	1.00	0.008	1.00	7.15
LYS115	HD3	1.00	0.005	1.00	7.15
LYS115	HE2	1.00	0.008	1.00	220.78

3.115.6 Detailed Probabilities of LYS115N:

Overall probability: 0.916

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU114	0.86	1.00
LYS115	0.97	1.00
ILE116	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L114HA	1.00
L114H	1.00
L114HB3	1.00
L114HB2	1.00
L114HG	0.98
K115HA	1.00
K115HB2	1.00
K115HB3	1.00
K115HG2	1.00
K115HG3	1.00
K115H	1.00
I116H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU114	HA	1.00	0.001	1.00	-298211.00
LEU114	HB2	1.00	0.011	1.00	-509652.00
LEU114	HB3	1.00	0.014	1.00	-388179.00
LEU114	HG	0.98	0.095	0.02	0.00
LEU114	H	1.00	0.005	1.00	-990666.00
LEU114	HD11	0.52	0.009	1.00	-202653.00
LEU114	HD21	0.59	0.007	1.00	-232572.00
LYS115	HA	1.00	0.002	1.00	-867318.00
LYS115	HB2	1.00	0.026	1.00	-1317662.00
LYS115	HB3	1.00	0.032	0.80	0.00
LYS115	HG2	1.00	0.013	1.00	-3332692.00
LYS115	HG3	1.00	0.000	1.00	-235878.00
LYS115	H	1.00	0.027	1.00	-19107776.00
ILE116	H	1.00	0.002	1.00	-883825.00

3.115.7 Detailed Probabilities of LYS115HA:

Overall probability: 0.929

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU114	0.75	1.00
LYS115	1.00	1.00
ILE116	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L114HA	1.00
K115HB2	1.00
K115HB3	1.00
K115HG2	1.00
K115HG3	1.00
K115HD2	0.98
K115HD3	0.98
K115H	1.00
K115HA	1.00
I116HA	1.00
I116H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU114	HA	1.00	0.091	0.00	0.00
LEU114	HB2	0.70	0.013	1.00	0.65
LEU114	HB3	0.90	0.016	1.00	0.66
LEU114	H	0.89	0.003	1.00	-251903.00
LYS115	HA	1.00	0.000	1.00	13.14
LYS115	HB2	1.00	0.021	1.00	2.44
LYS115	HB3	1.00	0.021	1.00	2.44
LYS115	HG2	1.00	0.003	1.00	0.84
LYS115	HG3	1.00	0.004	1.00	0.46
LYS115	HD2	0.98	0.009	1.00	0.59
LYS115	HD3	0.98	0.009	1.00	0.59
LYS115	H	1.00	0.002	1.00	-867318.00
ILE116	HA	1.00	0.010	1.00	0.07
ILE116	H	1.00	0.001	1.00	-405817.00

3.115.8 Detailed Probabilities of LYS115HB2:

Overall probability: 0.909

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS115	0.89	1.00
ILE116	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K115HA	1.00
K115HB3	1.00
K115HG2	1.00
K115HG3	1.00
K115HD2	1.00
K115HD3	1.00
K115HE2	0.98
K115H	1.00
K115HB2	1.00
I116H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS115	HA	1.00	0.370	0.00	0.00
LYS115	HB2	1.00	0.024	1.00	53.87
LYS115	HB3	1.00	0.024	1.00	53.87
LYS115	HG2	1.00	0.010	1.00	2.64
LYS115	HG3	1.00	0.013	1.00	1.00
LYS115	HD2	1.00	0.004	1.00	5.45
LYS115	HD3	1.00	0.004	1.00	5.45
LYS115	HE2	0.98	0.013	1.00	1.28
LYS115	H	1.00	0.026	1.00	-1317662.00
ILE116	H	1.00	0.008	1.00	-631174.00
ILE116	HA	0.67	0.008	1.00	0.07

3.115.9 Detailed Probabilities of LYS115HB3:

Overall probability: 0.891

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS115	0.87	1.00
ILE116	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K115HA	1.00
K115HB2	1.00
K115HG2	1.00
K115HG3	1.00
K115HD2	1.00
K115HD3	1.00
K115HE2	0.99
K115H	1.00
K115HB3	1.00
I116H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS115	HA	1.00	0.376	0.00	0.00
LYS115	HB2	1.00	0.030	1.00	0.00
LYS115	HB3	1.00	0.030	1.00	0.00
LYS115	HG2	1.00	0.016	1.00	2.64
LYS115	HG3	1.00	0.007	1.00	1.00
LYS115	HD2	1.00	0.002	1.00	5.45
LYS115	HD3	1.00	0.002	1.00	5.45
LYS115	HE2	0.99	0.019	1.00	1.28
LYS115	H	1.00	0.032	0.80	0.00
ILE116	H	1.00	0.002	1.00	-631174.00
ILE116	HA	0.85	0.014	1.00	0.07

3.115.10 Detailed Probabilities of LYS115HG2:

Overall probability: 0.703

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS115	0.78	0.90
ILE116	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
K115HA	1.00
K115HB2	1.00
K115HB3	1.00
K115HG3	1.00
K115HD2	1.00
K115HD3	1.00
K115HE2	1.00
K115H	1.00
K115HZ2	1.00
K115HG2	1.00
I116H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS115	HA	1.00	0.003	1.00	0.96
LYS115	HB2	1.00	0.022	1.00	3.20
LYS115	HB3	1.00	0.022	1.00	3.20
LYS115	HG2	1.00	0.001	1.00	37.64
LYS115	HG3	1.00	0.003	1.00	5.34
LYS115	HD2	1.00	0.158	0.00	0.00
LYS115	HD3	1.00	0.158	0.00	0.00
LYS115	HE2	1.00	0.001	1.00	1.96
LYS115	H	1.00	0.013	1.00	-3332692.00
ILE116	H	0.97	0.058	0.03	0.00

3.115.11 Detailed Probabilities of LYS115HG3:

Overall probability: 0.500

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS115	0.44	0.90
ILE116	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K115HA	1.00
K115HB2	1.00
K115HB3	1.00
K115HG2	1.00
K115HD2	1.00
K115HD3	1.00
K115HE2	1.00
K115H	1.00
K115HZ2	1.00
K115HG3	1.00
I116H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS115	HA	1.00	0.222	0.00	0.00
LYS115	HB2	1.00	0.283	0.00	0.00
LYS115	HB3	1.00	0.283	0.00	0.00
LYS115	HG2	1.00	0.016	1.00	5.85
LYS115	HG3	1.00	0.002	1.00	15.45
LYS115	HD2	1.00	0.103	0.00	0.00
LYS115	HD3	1.00	0.103	0.00	0.00
LYS115	HE2	1.00	0.009	1.00	0.77
LYS115	H	1.00	0.000	1.00	-235878.00
ILE116	H	0.96	0.006	1.00	-127419.00

3.115.12 Detailed Probabilities of LYS115HD2:

Overall probability: 0.752

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS115	0.75	0.89

Expected NOESY Contacts

Proton	Expected probability
K115HA	0.98
K115HB2	1.00
K115HB3	1.00
K115HG2	1.00
K115HG3	1.00
K115HD3	1.00
K115HE2	1.00
K115HZ2	1.00
K115HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS115	HA	0.98	0.098	0.02	0.00
LYS115	HB2	1.00	0.027	1.00	5.56
LYS115	HB3	1.00	0.027	1.00	5.56
LYS115	HG2	1.00	0.056	0.00	0.00
LYS115	HG3	1.00	0.002	1.00	2.37
LYS115	HD2	1.00	0.028	1.00	244.35
LYS115	HD3	1.00	0.028	1.00	244.35
LYS115	HE2	1.00	0.008	1.00	7.15

3.115.13 Detailed Probabilities of LYS115HD3:

Overall probability: 0.753

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS115	0.75	0.89

Expected NOESY Contacts

Proton	Expected probability
K115HA	0.98
K115HB2	1.00
K115HB3	1.00
K115HG2	1.00
K115HG3	1.00
K115HD2	1.00
K115HE2	1.00
K115HZ2	1.00
K115HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS115	HA	0.98	0.101	0.02	0.00
LYS115	HB2	1.00	0.024	1.00	5.56
LYS115	HB3	1.00	0.024	1.00	5.56
LYS115	HG2	1.00	0.059	0.00	0.00
LYS115	HG3	1.00	0.005	1.00	2.37
LYS115	HD2	1.00	0.025	1.00	244.35
LYS115	HD3	1.00	0.025	1.00	244.35
LYS115	HE2	1.00	0.005	1.00	7.15

3.115.14 Detailed Probabilities of LYS115HE2:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS115	1.00	0.88

Expected NOESY Contacts

Proton	Expected probability
K115HB2	0.98
K115HB3	0.99
K115HG2	1.00
K115HG3	1.00
K115HD2	1.00
K115HD3	1.00
K115HE3	1.00
K115HZ2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS115	HB2	0.99	0.020	1.00	0.70
LYS115	HB3	0.99	0.020	1.00	0.70
LYS115	HG2	1.00	0.018	1.00	1.05
LYS115	HG3	1.00	0.005	1.00	0.63
LYS115	HD2	1.00	0.004	1.00	4.26
LYS115	HD3	1.00	0.004	1.00	4.26
LYS115	HE2	1.00	0.008	1.00	220.78

3.115.15 Detailed Probabilities of LYS115H:

Overall probability: 0.939

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU114	0.86	1.00
LYS115	1.00	1.00
ILE116	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L114HA	1.00
L114H	1.00
L114HB3	1.00
L114HB2	1.00
L114HG	0.98
K115HA	1.00
K115HB2	1.00
K115HB3	1.00
K115HG2	1.00
K115HG3	1.00
K115H	1.00
I116H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU114	HA	1.00	0.011	1.00	0.18
LEU114	HB2	1.00	0.018	1.00	0.53
LEU114	HB3	1.00	0.025	1.00	0.66
LEU114	HG	0.98	0.135	0.02	0.00
LEU114	H	1.00	0.002	1.00	-808297.00
LEU114	HD11	0.52	0.014	1.00	0.35
LEU114	HD21	0.59	0.004	1.00	0.24
LYS115	HA	1.00	0.009	1.00	0.97
LYS115	HB2	1.00	0.002	1.00	2.14
LYS115	HB3	1.00	0.002	1.00	2.14
LYS115	HG2	1.00	0.003	1.00	0.53
LYS115	HG3	1.00	0.004	1.00	0.28
LYS115	H	1.00	0.027	1.00	-19107776.00
LYS115	HD2	0.88	0.002	1.00	0.43
LYS115	HD3	0.87	0.002	1.00	0.43
ILE116	H	1.00	0.003	1.00	-642492.00

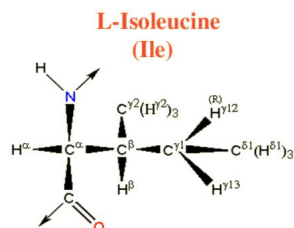


Figure 115: Image from the BMRB

Residue probability: 0.807
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	177.016	175.926	2.710	0.000	0.000
CA 3.116.1	64.122	61.717	4.152	0.923	1.000
CB 3.116.2	36.323	38.702	3.945	0.875	1.000
CG1 3.116.3	28.888	27.785	2.037	0.750	1.000
CG2 3.116.4	18.105	17.574	1.928	0.889	1.000
CD1 3.116.5	13.410	13.545	3.646	0.714	1.000
N 3.116.6	120.613	121.467	6.098	0.895	1.000
HA 3.116.7	3.460	4.185	1.403	0.818	1.000
HB 3.116.8	1.630	1.776	0.310	0.667	1.000
HG12 3.116.9	1.584	1.271	0.411	0.315	1.000
HG13 3.116.10	0.970	1.186	0.426	0.857	1.000
HG2 3.116.11	0.043	0.762	0.283	1.000	1.000
HD1 3.116.12	0.680	0.668	0.293	0.857	1.000
H 3.116.13	8.004	8.301	0.685	0.932	1.000

3.116.1 Detailed Probabilities of ILE116CA:

Overall probability: 0.923
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS115	1.00	1.00
ILE116	1.00	1.00
VAL117	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
K115HA	1.00
I116HB	1.00
I116HG12	1.00
I116HG13	1.00
I116HG21	1.00
I116HD11	0.97
I116H	1.00
I116HA	1.00
V117HA	1.00
V117H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS115	HA	1.00	0.010	1.00	0.07
LYS115	HB2	0.67	0.008	1.00	0.07
LYS115	HB3	0.85	0.014	1.00	0.07
ILE116	HA	1.00	0.002	1.00	3.84
ILE116	HB	1.00	0.025	1.00	0.49
ILE116	HG12	1.00	0.021	1.00	0.49
ILE116	HG13	1.00	0.004	1.00	0.42
ILE116	HG21	1.00	0.001	1.00	0.61
ILE116	HD11	0.97	0.001	1.00	0.38
ILE116	H	1.00	0.009	1.00	0.37
VAL117	HA	1.00	0.202	0.00	0.00
VAL117	H	1.00	0.000	1.00	0.13
VAL117	HG21	0.53	0.003	1.00	0.10

3.116.2 Detailed Probabilities of ILE116CB:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE116	0.86	1.00
VAL117	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I116HA	1.00
I116HG12	1.00
I116HG13	1.00
I116HG21	1.00
I116HD11	1.00
I116H	1.00
I116HB	1.00
V117H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE116	HA	1.00	0.005	1.00	0.23
ILE116	HB	1.00	0.002	1.00	2.04
ILE116	HG12	1.00	0.048	0.00	0.00
ILE116	HG13	1.00	0.003	1.00	0.20
ILE116	HG21	1.00	0.001	1.00	0.63
ILE116	HD11	1.00	0.003	1.00	0.61
ILE116	H	1.00	0.010	1.00	0.54
VAL117	H	1.00	0.002	1.00	0.30

3.116.3 Detailed Probabilities of ILE116CG1:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE116	0.71	1.00
VAL117	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I116HA	1.00
I116HB	1.00
I116HG13	1.00
I116HG21	1.00
I116HD11	1.00
I116H	1.00
I116HG12	1.00
V117H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE116	HA	1.00	0.004	1.00	0.33
ILE116	HB	1.00	0.355	0.00	0.00
ILE116	HG12	1.00	0.309	0.00	0.00
ILE116	HG13	1.00	0.004	1.00	1.60
ILE116	HG21	1.00	0.001	1.00	0.33
ILE116	HD11	1.00	0.001	1.00	0.95
ILE116	H	1.00	0.002	1.00	0.48
VAL117	H	0.98	0.001	1.00	0.07

3.116.4 Detailed Probabilities of ILE116CG2:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE116	0.86	1.00
VAL117	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I116HA	1.00
I116HB	1.00
I116HG12	1.00
I116HG13	1.00
I116HG22	1.00
I116HD11	0.99
I116H	1.00
V117H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE116	HA	1.00	0.005	1.00	0.48
ILE116	HB	1.00	0.002	1.00	0.78
ILE116	HG12	1.00	0.044	0.00	0.00
ILE116	HG13	1.00	0.005	1.00	0.39
ILE116	HG21	1.00	0.001	1.00	12.63
ILE116	HD11	0.99	0.005	1.00	1.18
ILE116	H	1.00	0.015	1.00	0.19
VAL117	H	0.99	0.007	1.00	0.18
VAL117	HA	0.67	0.000	1.00	0.08

3.116.5 Detailed Probabilities of ILE116CD1:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE116	0.71	1.00

Expected NOESY Contacts

Proton	Expected probability
I116HA	0.97
I116HB	1.00
I116HG12	1.00
I116HG13	1.00
I116HG21	0.99
I116HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE116	HA	0.97	0.009	1.00	0.43
ILE116	HB	1.00	0.262	0.00	0.00
ILE116	HG12	1.00	0.216	0.00	0.00
ILE116	HG13	1.00	0.004	1.00	1.59
ILE116	HG21	0.99	0.001	1.00	1.68
ILE116	HD11	1.00	0.008	1.00	59.32
ILE116	H	0.94	0.005	1.00	0.38

3.116.6 Detailed Probabilities of ILE116N:

Overall probability: 0.895

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS115	0.84	1.00
ILE116	0.93	1.00
VAL117	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K115H	1.00
K115HG2	0.97
K115HG3	0.96
K115HA	1.00
K115HB2	1.00
K115HB3	1.00
I116HA	1.00
I116HB	1.00
I116HG12	1.00
I116HG13	1.00
I116HG21	1.00
I116H	1.00
V117H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS115	HA	1.00	0.001	1.00	-405817.00
LYS115	HB2	1.00	0.008	1.00	-631174.00
LYS115	HB3	1.00	0.002	1.00	-631174.00
LYS115	HG2	0.97	0.058	0.03	0.00
LYS115	HG3	0.96	0.006	1.00	-127419.00
LYS115	H	1.00	0.003	1.00	-642492.00
ILE116	HA	1.00	0.001	1.00	-499676.00
ILE116	HB	1.00	0.011	1.00	-1323370.00
ILE116	HG12	1.00	0.035	0.50	0.00
ILE116	HG13	1.00	0.005	1.00	-514257.00
ILE116	HG21	1.00	0.001	1.00	-339550.00
ILE116	H	1.00	0.002	1.00	-5371222.00
ILE116	HD11	0.94	0.003	1.00	-519532.00
VAL117	H	1.00	0.000	1.00	-767490.00

3.116.7 Detailed Probabilities of ILE116HA:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS115	0.00	1.00
ILE116	1.00	1.00
VAL117	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
K115HA	1.00
I116HB	1.00
I116HG12	1.00
I116HG13	1.00
I116HG21	1.00
I116HD11	0.97
I116H	1.00
I116HA	1.00
V117HA	1.00
V117H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS115	HA	1.00	0.304	0.00	0.00
ILE116	HA	1.00	0.002	1.00	3.84
ILE116	HB	1.00	0.005	1.00	0.23
ILE116	HG12	1.00	0.004	1.00	0.33
ILE116	HG13	1.00	0.000	1.00	0.40
ILE116	HG21	1.00	0.005	1.00	0.48
ILE116	HD11	0.97	0.009	1.00	0.43
ILE116	H	1.00	0.001	1.00	-499676.00
VAL117	HA	1.00	0.198	0.00	0.00
VAL117	H	1.00	0.005	1.00	-199285.00
VAL117	HG21	0.53	0.022	1.00	0.06

3.116.8 Detailed Probabilities of ILE116HB:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE116	0.57	1.00
VAL117	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I116HA	1.00
I116HG12	1.00
I116HG13	1.00
I116HG21	1.00
I116HD11	1.00
I116H	1.00
I116HB	1.00
V117H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE116	HA	1.00	0.025	1.00	0.49
ILE116	HB	1.00	0.002	1.00	2.04
ILE116	HG12	1.00	0.355	0.00	0.00
ILE116	HG13	1.00	0.040	0.00	0.00
ILE116	HG21	1.00	0.002	1.00	0.78
ILE116	HD11	1.00	0.262	0.00	0.00
ILE116	H	1.00	0.011	1.00	-1323370.00
VAL117	H	1.00	0.001	1.00	-892233.00
VAL117	HA	0.89	0.006	1.00	0.06

3.116.9 Detailed Probabilities of ILE116HG12:

Overall probability: 0.315

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE116	0.36	1.00
VAL117	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
I116HA	1.00
I116HB	1.00
I116HG13	1.00
I116HG21	1.00
I116HD11	1.00
I116H	1.00
I116HG12	1.00
V117H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE116	HA	1.00	0.021	1.00	0.49
ILE116	HB	1.00	0.048	0.00	0.00
ILE116	HG12	1.00	0.309	0.00	0.00
ILE116	HG13	1.00	0.006	1.00	1.62
ILE116	HG21	1.00	0.044	0.00	0.00
ILE116	HD11	1.00	0.216	0.00	0.00
ILE116	H	1.00	0.035	0.50	0.00
VAL117	H	0.98	0.047	0.02	0.00

3.116.10 Detailed Probabilities of ILE116HG13:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE116	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
I116HA	1.00
I116HB	1.00
I116HG12	1.00
I116HG21	1.00
I116HD11	1.00
I116H	1.00
I116HG13	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE116	HA	1.00	0.004	1.00	0.42
ILE116	HB	1.00	0.003	1.00	0.20
ILE116	HG12	1.00	0.004	1.00	1.60
ILE116	HG13	1.00	0.172	0.00	0.00
ILE116	HG21	1.00	0.005	1.00	0.39
ILE116	HD11	1.00	0.004	1.00	1.59
ILE116	H	1.00	0.005	1.00	-514257.00

3.116.11 Detailed Probabilities of ILE116HG21:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE116	1.00	1.00
VAL117	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I116HA	1.00
I116HB	1.00
I116HG12	1.00
I116HG13	1.00
I116HG22	1.00
I116HD11	0.99
I116H	1.00
V117H	0.99

NOESY contacts detailed probability

3.116 ILE(116)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE116	HA	1.00	0.001	1.00	0.61
ILE116	HB	1.00	0.001	1.00	0.63
ILE116	HG12	1.00	0.001	1.00	0.33
ILE116	HG13	1.00	0.001	1.00	0.41
ILE116	HG21	1.00	0.001	1.00	12.63
ILE116	HD11	0.99	0.001	1.00	1.68
ILE116	H	1.00	0.001	1.00	-339550.00
VAL117	H	0.99	0.002	1.00	-385811.00
VAL117	HA	0.67	0.003	1.00	0.17

3.116.12 Detailed Probabilities of ILE116HD11:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE116	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
I116HA	0.97
I116HB	1.00
I116HG12	1.00
I116HG13	1.00
I116HG21	0.99
I116HD12	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE116	HA	0.97	0.001	1.00	0.38
ILE116	HB	1.00	0.003	1.00	0.61
ILE116	HG12	1.00	0.001	1.00	0.95
ILE116	HG13	1.00	0.118	0.00	0.00
ILE116	HG21	0.99	0.005	1.00	1.18
ILE116	HD11	1.00	0.008	1.00	59.32
ILE116	H	0.94	0.003	1.00	-519532.00

3.116.13 Detailed Probabilities of ILE116H:

Overall probability: 0.932

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS115	0.86	1.00
ILE116	1.00	1.00
VAL117	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K115H	1.00
K115HG2	0.97
K115HG3	0.96
K115HA	1.00
K115HB2	1.00
K115HB3	1.00
I116HA	1.00
I116HB	1.00
I116HG12	1.00
I116HG13	1.00
I116HG21	1.00
I116H	1.00
V117H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS115	HA	1.00	0.027	1.00	0.77
LYS115	HB2	1.00	0.027	1.00	1.13
LYS115	HB3	1.00	0.027	1.00	1.13
LYS115	HG2	0.97	0.032	0.80	0.00
LYS115	HG3	0.96	0.173	0.04	0.00
LYS115	H	1.00	0.002	1.00	-883825.00
LYS115	HD2	0.54	0.030	1.00	0.00
LYS115	HD3	0.55	0.030	1.00	0.00
ILE116	HA	1.00	0.009	1.00	0.37
ILE116	HB	1.00	0.010	1.00	0.54
ILE116	HG12	1.00	0.002	1.00	0.48
ILE116	HG13	1.00	0.003	1.00	0.39
ILE116	HG21	1.00	0.015	1.00	0.19
ILE116	H	1.00	0.002	1.00	-5371222.00
ILE116	HD11	0.94	0.005	1.00	0.38
VAL117	H	1.00	0.024	1.00	-1466097.00
VAL117	HA	0.92	0.025	1.00	0.19

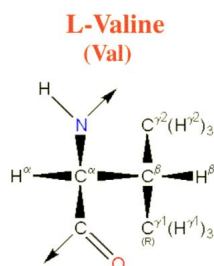


Figure 116: Image from the BMRB

Residue probability: 0.733
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	177.746	175.682	2.367	0.000	0.000
CA 3.117.1	67.505	62.613	4.828	0.818	1.000
CB 3.117.2	30.753	32.918	4.591	0.667	1.000
CG1 3.117.3	21.310	21.563	2.746	0.338	1.000
CG2 3.117.4	23.986	21.368	2.801	0.780	1.000
N 3.117.5	120.234	121.057	5.832	0.925	1.000
HA 3.117.6	3.260	4.178	0.599	0.778	1.000
HB 3.117.7	2.047	1.980	0.322	0.857	1.000
HG1 3.117.8	0.721	0.816	0.264	0.833	1.000
HG2 3.117.9	0.865	0.803	0.504	0.580	1.000
H 3.117.10	8.121	8.311	0.669	0.750	1.000

3.117.1 Detailed Probabilities of VAL117CA:

Overall probability: 0.818
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE116	0.75	1.00
VAL117	1.00	1.00
ARG118	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
I116HA	1.00
V117HG11	1.00
V117HG21	1.00
V117H	1.00
V117HB	1.00
V117HA	1.00
R118HA	1.00
R118H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE116	HA	1.00	0.198	0.00	0.00
ILE116	HB	0.89	0.006	1.00	0.06
ILE116	HG21	0.67	0.003	1.00	0.17
ILE116	H	0.92	0.025	1.00	0.19
VAL117	HA	1.00	0.002	1.00	4.70
VAL117	HB	1.00	0.010	1.00	0.35
VAL117	HG11	1.00	0.008	1.00	1.01
VAL117	HG21	1.00	0.005	1.00	1.16
VAL117	H	1.00	0.008	1.00	0.50
ARG118	HA	1.00	0.076	0.00	0.00
ARG118	H	1.00	0.003	1.00	0.19

3.117.2 Detailed Probabilities of VAL117CB:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL117	0.60	1.00
ARG118	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V117HA	1.00
V117HG11	1.00
V117HG21	1.00
V117H	1.00
V117HB	1.00
R118H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL117	HA	1.00	0.002	1.00	0.27
VAL117	HB	1.00	0.452	0.00	0.00
VAL117	HG11	1.00	0.007	1.00	1.49
VAL117	HG21	1.00	0.598	0.00	0.00
VAL117	H	1.00	0.009	1.00	0.91
ARG118	H	1.00	0.000	1.00	0.45

3.117.3 Detailed Probabilities of VAL117CG1:

Overall probability: 0.338

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL117	0.40	1.00
ARG118	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
V117HA	1.00
V117HG12	1.00
V117HG21	1.00
V117H	1.00
V117HB	1.00
R118H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL117	HA	1.00	0.000	1.00	0.93
VAL117	HB	1.00	0.010	1.00	1.87
VAL117	HG11	1.00	0.286	0.00	0.00
VAL117	HG21	1.00	0.430	0.00	0.00
VAL117	H	1.00	0.203	0.00	0.00
ARG118	H	0.97	0.298	0.03	0.00

3.117.4 Detailed Probabilities of VAL117CG2:

Overall probability: 0.780

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL117	0.78	1.00

Expected NOESY Contacts

Proton	Expected probability
V117HA	1.00
V117HG11	1.00
V117HG22	1.00
V117H	1.00
V117HB	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL117	HA	1.00	0.001	1.00	1.35
VAL117	HB	1.00	0.007	1.00	1.53
VAL117	HG11	1.00	0.010	1.00	6.88
VAL117	HG21	1.00	0.031	0.90	0.00
VAL117	H	1.00	1.332	0.00	0.00

3.117.5 Detailed Probabilities of VAL117N:

Overall probability: 0.925

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE116	0.84	1.00
VAL117	1.00	1.00
ARG118	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
I116HG21	0.99
I116HA	1.00
I116H	1.00
I116HG12	0.98
I116HB	1.00
V117HA	1.00
V117HG11	1.00
V117HG21	1.00
V117HB	1.00
V117H	1.00
R118H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE116	HA	1.00	0.005	1.00	-199285.00
ILE116	HB	1.00	0.001	1.00	-892233.00
ILE116	HG12	0.98	0.047	0.02	0.00
ILE116	HG21	0.99	0.002	1.00	-385811.00
ILE116	H	1.00	0.024	1.00	-1466097.00
ILE116	HG13	0.92	0.013	1.00	-143441.00
VAL117	HA	1.00	0.030	1.00	0.00
VAL117	HB	1.00	0.008	1.00	-2103946.00
VAL117	HG11	1.00	0.029	1.00	-903569.00
VAL117	HG21	1.00	0.002	1.00	-2339844.00
VAL117	H	1.00	0.008	1.00	-16420475.00
ARG118	H	1.00	0.002	1.00	-1466097.00
ARG118	HA	0.92	0.012	1.00	-608202.00

3.117.6 Detailed Probabilities of VAL117HA:

Overall probability: 0.778

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE116	0.50	1.00
VAL117	1.00	1.00
ARG118	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
I116HA	1.00
V117HG11	1.00
V117HG21	1.00
V117H	1.00
V117HB	1.00
V117HA	1.00
R118HA	1.00
R118H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE116	HA	1.00	0.202	0.00	0.00
ILE116	HG21	0.67	0.000	1.00	0.08
VAL117	HA	1.00	0.002	1.00	4.70
VAL117	HB	1.00	0.002	1.00	0.27
VAL117	HG11	1.00	0.000	1.00	0.93
VAL117	HG21	1.00	0.001	1.00	1.35
VAL117	H	1.00	0.030	1.00	0.00
ARG118	HA	1.00	0.106	0.00	0.00
ARG118	H	1.00	0.008	1.00	-135406.00

3.117.7 Detailed Probabilities of VAL117HB:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL117	0.80	1.00
ARG118	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V117HA	1.00
V117HG11	1.00
V117HG21	1.00
V117H	1.00
V117HB	1.00
R118H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL117	HA	1.00	0.010	1.00	0.35
VAL117	HB	1.00	0.452	0.00	0.00
VAL117	HG11	1.00	0.010	1.00	1.87
VAL117	HG21	1.00	0.007	1.00	1.53
VAL117	H	1.00	0.008	1.00	-2103946.00
ARG118	H	1.00	0.009	1.00	-914064.00
ARG118	HA	0.82	0.023	1.00	0.44

3.117.8 Detailed Probabilities of VAL117HG11:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL117	0.80	1.00
ARG118	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V117HA	1.00
V117HG12	1.00
V117HG21	1.00
V117H	1.00
V117HB	1.00
R118H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL117	HA	1.00	0.008	1.00	1.01
VAL117	HB	1.00	0.007	1.00	1.49
VAL117	HG11	1.00	0.286	0.00	0.00
VAL117	HG21	1.00	0.010	1.00	6.88
VAL117	H	1.00	0.029	1.00	-903569.00
ARG118	H	0.98	0.027	1.00	-670529.00

3.117.9 Detailed Probabilities of VAL117HG21:

Overall probability: 0.580

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL117	0.58	1.00

Expected NOESY Contacts

Proton	Expected probability
V117HA	1.00
V117HG11	1.00
V117HG22	1.00
V117H	1.00
V117HB	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL117	HA	1.00	0.005	1.00	1.16
VAL117	HB	1.00	0.598	0.00	0.00
VAL117	HG11	1.00	0.430	0.00	0.00
VAL117	HG21	1.00	0.031	0.90	0.00
VAL117	H	1.00	0.002	1.00	-2339844.00

3.117.10 Detailed Probabilities of VAL117H:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ILE116	1.00	1.00
VAL117	0.60	1.00
ARG118	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
I116HG21	0.99
I116HA	1.00
I116H	1.00
I116HG12	0.98
I116HB	1.00
V117HA	1.00
V117HG11	1.00
V117HG21	1.00
V117HB	1.00
V117H	1.00
R118H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ILE116	HA	1.00	0.000	1.00	0.13
ILE116	HB	1.00	0.002	1.00	0.30
ILE116	HG12	0.98	0.001	1.00	0.07
ILE116	HG21	0.99	0.007	1.00	0.18
ILE116	H	1.00	0.000	1.00	-767490.00
VAL117	HA	1.00	0.008	1.00	0.50
VAL117	HB	1.00	0.009	1.00	0.91
VAL117	HG11	1.00	0.203	0.00	0.00
VAL117	HG21	1.00	1.332	0.00	0.00
VAL117	H	1.00	0.008	1.00	-16420475.00
ARG118	H	1.00	0.078	0.00	0.00
ARG118	HA	0.92	0.015	1.00	0.15

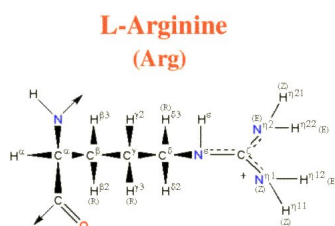
3.118 ARG(118)

Figure 117: Image from the BMRB

Residue probability: 0.633

Residue probability confidence: 0.912

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.966	176.453	2.303	0.000	0.000
CA 3.118.1	60.169	56.803	3.326	0.523	1.000
CB 3.118.2	29.702	30.892	2.424	0.636	1.000
CG 3.118.3	28.010	27.247	1.538	0.553	0.909
CD 3.118.4	43.758	43.189	1.415	0.889	0.800
N 3.118.5	118.415	120.701	3.779	0.740	1.000
NE 3.118.6	85.297	89.115	13.484	0.875	0.778
NH1	NA	—	—	0.000	0.000
NH2	NA	—	—	0.000	0.000
HA 3.118.7	3.893	4.301	0.495	0.667	1.000
HB2 3.118.8	1.799	1.793	0.292	0.300	1.000
HB3 3.118.9	1.871	1.757	0.307	0.520	1.000
HG2 3.118.10	1.729	1.559	0.294	0.402	0.909
HG3 3.118.11	1.483	1.535	0.310	0.700	0.909
HD2 3.118.12	3.151	3.105	0.301	0.689	0.800
HD3 3.118.13	2.971	3.081	0.306	0.778	0.800
H 3.118.14	8.026	8.248	0.623	0.716	1.000
HE 3.118.15	7.666	7.398	0.718	0.500	0.778
HH1	NA	—	—	0.000	0.000
HH2	NA	—	—	0.000	0.000

3.118.1 Detailed Probabilities of ARG118CA:

Overall probability: 0.523

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL117	0.67	1.00
ARG118	0.48	1.00
GLU119	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
V117HA	1.00
R118HB2	1.00
R118HB3	1.00
R118HG2	1.00
R118HG3	1.00
R118HD2	0.98
R118HD3	0.97
R118H	1.00
R118HA	1.00
E119HA	1.00
E119H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL117	HA	1.00	0.106	0.00	0.00
VAL117	HB	0.82	0.023	1.00	0.44
VAL117	H	0.92	0.015	1.00	0.15
ARG118	HA	1.00	0.268	0.00	0.00
ARG118	HB2	1.00	0.037	0.30	0.00
ARG118	HB3	1.00	0.035	0.50	0.00
ARG118	HG2	1.00	0.107	0.00	0.00
ARG118	HG3	1.00	0.353	0.00	0.00
ARG118	HD2	0.98	0.003	1.00	0.09
ARG118	HD3	0.97	0.004	1.00	0.07
ARG118	H	1.00	0.004	1.00	0.47
GLU119	HA	1.00	0.172	0.00	0.00
GLU119	H	1.00	0.005	1.00	0.30

3.118.2 Detailed Probabilities of ARG118CB:

Overall probability: 0.636

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG118	0.56	1.00
GLU119	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R118HA	1.00
R118HB2	1.00
R118HG2	1.00
R118HG3	1.00
R118HD2	1.00
R118HD3	1.00
R118H	1.00
R118HE	1.00
R118HB3	1.00
E119H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG118	HA	1.00	0.011	1.00	0.59
ARG118	HB2	1.00	0.105	0.00	0.00
ARG118	HB3	1.00	0.017	1.00	9.06
ARG118	HG2	1.00	0.009	1.00	4.77
ARG118	HG3	1.00	0.018	1.00	0.26
ARG118	HD2	1.00	0.070	0.00	0.00
ARG118	HD3	1.00	0.011	1.00	0.12
ARG118	H	1.00	0.061	0.00	0.00
ARG118	HE	1.00	0.124	0.00	0.00
GLU119	H	1.00	0.005	1.00	0.17
GLU119	HA	0.79	0.015	1.00	0.54

3.118.3 Detailed Probabilities of ARG118CG:

Overall probability: 0.553

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG118	0.61	0.90
GLU119	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
R118HA	1.00
R118HB2	1.00
R118HB3	1.00
R118HG2	1.00
R118HD2	1.00
R118HD3	1.00
R118H	1.00
R118HE	1.00
R118HH11	1.00
R118HG3	1.00
E119H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG118	HA	1.00	0.011	1.00	0.27
ARG118	HB2	1.00	0.035	0.50	0.00
ARG118	HB3	1.00	0.025	1.00	0.65
ARG118	HG2	1.00	0.105	0.00	0.00
ARG118	HG3	1.00	0.024	1.00	12.32
ARG118	HD2	1.00	0.001	1.00	0.25
ARG118	HD3	1.00	0.003	1.00	0.25
ARG118	H	1.00	0.520	0.00	0.00
ARG118	HE	1.00	0.880	0.00	0.00
GLU119	H	0.97	0.628	0.03	0.00

3.118.4 Detailed Probabilities of ARG118CD:

Overall probability: 0.889

Overall confidence: 0.800

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG118	0.89	0.80

Expected NOESY Contacts

Proton	Expected probability
R118HA	0.97
R118HB2	1.00
R118HB3	1.00
R118HG2	1.00
R118HG3	1.00
R118HD2	1.00
R118HE	1.00
R118HH11	1.00
R118HH21	1.00
R118HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG118	HA	0.97	0.003	1.00	0.12
ARG118	HB2	1.00	0.024	1.00	0.41
ARG118	HB3	1.00	0.048	0.00	0.00
ARG118	HG2	1.00	0.019	1.00	0.64
ARG118	HG3	1.00	0.003	1.00	0.34
ARG118	HD2	1.00	0.003	1.00	1.88
ARG118	HD3	1.00	0.001	1.00	7.85
ARG118	HE	1.00	0.000	1.00	0.15
ARG118	H	0.86	0.005	1.00	0.16

3.118.5 Detailed Probabilities of ARG118N:

Overall probability: 0.740

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL117	0.80	1.00
ARG118	0.79	1.00
GLU119	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V117HG11	0.98
V117H	1.00
V117HB	1.00
V117HA	1.00
R118HA	1.00
R118HB2	1.00
R118HB3	1.00
R118HG2	1.00
R118HG3	1.00
R118H	1.00
E119H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL117	HA	1.00	0.008	1.00	-135406.00
VAL117	HB	1.00	0.009	1.00	-914064.00
VAL117	HG11	0.98	0.027	1.00	-670529.00
VAL117	H	1.00	0.078	0.00	0.00
VAL117	HG21	0.94	0.006	1.00	-1360443.00
ARG118	HA	1.00	0.008	1.00	-628522.00
ARG118	HB2	1.00	0.030	1.00	0.00
ARG118	HB3	1.00	0.039	0.10	0.00
ARG118	HG2	1.00	0.040	0.00	0.00
ARG118	HG3	1.00	0.005	1.00	-448311.00
ARG118	H	1.00	0.017	1.00	-14033966.00
ARG118	HD2	0.87	0.021	1.00	-97393.00
ARG118	HD3	0.86	0.004	1.00	-107980.00
ARG118	HE	0.59	0.024	1.00	-697715.00
GLU119	H	1.00	0.106	0.00	0.00

3.118.6 Detailed Probabilities of ARG118NE:

Overall probability: 0.875

Overall confidence: 0.778

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG118	0.88	0.78

Expected NOESY Contacts

Proton	Expected probability
R118HB2	1.00
R118HB3	1.00
R118HG2	1.00
R118HG3	1.00
R118HD2	1.00
R118HD3	1.00
R118HH11	1.00
R118HH21	1.00
R118HE	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG118	HB2	1.00	0.047	0.00	0.00
ARG118	HB3	1.00	0.025	1.00	-144066.00
ARG118	HG2	1.00	0.004	1.00	-180479.00
ARG118	HG3	1.00	0.003	1.00	-186569.00
ARG118	HD2	1.00	0.003	1.00	-254288.00
ARG118	HD3	1.00	0.002	1.00	-249416.00
ARG118	HE	1.00	0.005	1.00	-1884892.00
ARG118	H	0.59	0.021	1.00	-70142.00

3.118.7 Detailed Probabilities of ARG118HA:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL117	0.50	1.00
ARG118	0.75	1.00
GLU119	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
V117HA	1.00
R118HB2	1.00
R118HB3	1.00
R118HG2	1.00
R118HG3	1.00
R118HD2	0.98
R118HD3	0.97
R118H	1.00
R118HA	1.00
E119HA	1.00
E119H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL117	HA	1.00	0.076	0.00	0.00
VAL117	H	0.92	0.012	1.00	-608202.00
ARG118	HA	1.00	0.268	0.00	0.00
ARG118	HB2	1.00	0.099	0.00	0.00
ARG118	HB3	1.00	0.011	1.00	0.59
ARG118	HG2	1.00	0.007	1.00	0.22
ARG118	HG3	1.00	0.011	1.00	0.27
ARG118	HD2	0.98	0.003	1.00	0.12
ARG118	HD3	0.97	0.003	1.00	0.12
ARG118	H	1.00	0.008	1.00	-628522.00
GLU119	HA	1.00	0.080	0.00	0.00
GLU119	H	1.00	0.003	1.00	-191191.00

3.118.8 Detailed Probabilities of ARG118HB2:

Overall probability: 0.300

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG118	0.33	1.00
GLU119	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R118HA	1.00
R118HB3	1.00
R118HG2	1.00
R118HG3	1.00
R118HD2	1.00
R118HD3	1.00
R118H	1.00
R118HE	1.00
R118HB2	1.00
E119H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG118	HA	1.00	0.037	0.30	0.00
ARG118	HB2	1.00	0.606	0.00	0.00
ARG118	HB3	1.00	0.105	0.00	0.00
ARG118	HG2	1.00	1.307	0.00	0.00
ARG118	HG3	1.00	0.035	0.50	0.00
ARG118	HD2	1.00	0.038	0.20	0.00
ARG118	HD3	1.00	0.024	1.00	0.41
ARG118	H	1.00	0.030	1.00	0.00
ARG118	HE	1.00	0.047	0.00	0.00
GLU119	H	1.00	0.096	0.00	0.00

3.118.9 Detailed Probabilities of ARG118HB3:

Overall probability: 0.520

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG118	0.47	1.00
GLU119	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R118HA	1.00
R118HB2	1.00
R118HG2	1.00
R118HG3	1.00
R118HD2	1.00
R118HD3	1.00
R118H	1.00
R118HE	1.00
R118HB3	1.00
E119H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG118	HA	1.00	0.035	0.50	0.00
ARG118	HB2	1.00	0.678	0.00	0.00
ARG118	HB3	1.00	0.017	1.00	9.06
ARG118	HG2	1.00	1.235	0.00	0.00
ARG118	HG3	1.00	0.025	1.00	0.65
ARG118	HD2	1.00	0.034	0.60	0.00
ARG118	HD3	1.00	0.048	0.00	0.00
ARG118	H	1.00	0.039	0.10	0.00
ARG118	HE	1.00	0.025	1.00	-144066.00
GLU119	H	1.00	0.024	1.00	-1423236.00

3.118.10 Detailed Probabilities of ARG118HG2:

Overall probability: 0.402

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG118	0.44	0.90
GLU119	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
R118HA	1.00
R118HB2	1.00
R118HB3	1.00
R118HG3	1.00
R118HD2	1.00
R118HD3	1.00
R118H	1.00
R118HE	1.00
R118HH11	1.00
R118HG2	1.00
E119H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG118	HA	1.00	0.107	0.00	0.00
ARG118	HB2	1.00	0.536	0.00	0.00
ARG118	HB3	1.00	0.009	1.00	4.77
ARG118	HG2	1.00	1.377	0.00	0.00
ARG118	HG3	1.00	0.105	0.00	0.00
ARG118	HD2	1.00	0.020	1.00	0.54
ARG118	HD3	1.00	0.019	1.00	0.64
ARG118	H	1.00	0.040	0.00	0.00
ARG118	HE	1.00	0.004	1.00	-180479.00
GLU119	H	0.98	0.118	0.02	0.00

3.118.11 Detailed Probabilities of ARG118HG3:

Overall probability: 0.700

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG118	0.67	0.90
GLU119	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R118HA	1.00
R118HB2	1.00
R118HB3	1.00
R118HG2	1.00
R118HD2	1.00
R118HD3	1.00
R118H	1.00
R118HE	1.00
R118HH11	1.00
R118HG3	1.00
E119H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG118	HA	1.00	0.353	0.00	0.00
ARG118	HB2	1.00	0.290	0.00	0.00
ARG118	HB3	1.00	0.018	1.00	0.26
ARG118	HG2	1.00	1.623	0.00	0.00
ARG118	HG3	1.00	0.024	1.00	12.32
ARG118	HD2	1.00	0.000	1.00	0.48
ARG118	HD3	1.00	0.003	1.00	0.34
ARG118	H	1.00	0.005	1.00	-448311.00
ARG118	HE	1.00	0.003	1.00	-186569.00
GLU119	H	0.97	0.005	1.00	-114810.00

3.118.12 Detailed Probabilities of ARG118HD2:

Overall probability: 0.689

Overall confidence: 0.800

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG118	0.69	0.80

Expected NOESY Contacts

Proton	Expected probability
R118HA	0.98
R118HB2	1.00
R118HB3	1.00
R118HG2	1.00
R118HG3	1.00
R118HD3	1.00
R118HE	1.00
R118HH11	1.00
R118HH21	1.00
R118HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG118	HA	0.98	0.003	1.00	0.09
ARG118	HB2	1.00	0.038	0.20	0.00
ARG118	HB3	1.00	0.070	0.00	0.00
ARG118	HG2	1.00	0.004	1.00	0.27
ARG118	HG3	1.00	0.001	1.00	0.25
ARG118	HD2	1.00	0.100	0.00	0.00
ARG118	HD3	1.00	0.003	1.00	1.88
ARG118	HE	1.00	0.003	1.00	-254288.00
ARG118	H	0.87	0.021	1.00	-97393.00

3.118.13 Detailed Probabilities of ARG118HD3:

Overall probability: 0.778

Overall confidence: 0.800

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG118	0.78	0.80

Expected NOESY Contacts

Proton	Expected probability
R118HA	0.97
R118HB2	1.00
R118HB3	1.00
R118HG2	1.00
R118HG3	1.00
R118HD2	1.00
R118HE	1.00
R118HH11	1.00
R118HH21	1.00
R118HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG118	HA	0.97	0.004	1.00	0.07
ARG118	HB2	1.00	0.218	0.00	0.00
ARG118	HB3	1.00	0.011	1.00	0.12
ARG118	HG2	1.00	0.135	0.00	0.00
ARG118	HG3	1.00	0.003	1.00	0.25
ARG118	HD2	1.00	0.002	1.00	2.20
ARG118	HD3	1.00	0.001	1.00	7.85
ARG118	HE	1.00	0.002	1.00	-249416.00
ARG118	H	0.86	0.004	1.00	-107980.00

3.118.14 Detailed Probabilities of ARG118H:

Overall probability: 0.716

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
VAL117	0.76	1.00
ARG118	0.67	1.00
GLU119	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
V117HG11	0.98
V117H	1.00
V117HB	1.00
V117HA	1.00
R118HA	1.00
R118HB2	1.00
R118HB3	1.00
R118HG2	1.00
R118HG3	1.00
R118H	1.00
E119H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
VAL117	HA	1.00	0.003	1.00	0.19
VAL117	HB	1.00	0.000	1.00	0.45
VAL117	HG11	0.98	0.298	0.02	0.00
VAL117	H	1.00	0.002	1.00	-1466097.00
ARG118	HA	1.00	0.004	1.00	0.47
ARG118	HB2	1.00	0.001	1.00	0.19
ARG118	HB3	1.00	0.061	0.00	0.00
ARG118	HG2	1.00	1.767	0.00	0.00
ARG118	HG3	1.00	0.520	0.00	0.00
ARG118	H	1.00	0.017	1.00	-14033966.00
ARG118	HD2	0.87	0.003	1.00	0.14
ARG118	HD3	0.86	0.005	1.00	0.16
ARG118	HE	0.59	0.021	1.00	-70142.00
GLU119	H	1.00	0.003	1.00	-820448.00

3.118.15 Detailed Probabilities of ARG118HE:

Overall probability: 0.500

Overall confidence: 0.778

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG118	0.50	0.78

Expected NOESY Contacts

Proton	Expected probability
R118HB2	1.00
R118HB3	1.00
R118HG2	1.00
R118HG3	1.00
R118HD2	1.00
R118HD3	1.00
R118HH11	1.00
R118HH21	1.00
R118HE	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG118	HB2	1.00	0.256	0.00	0.00
ARG118	HB3	1.00	0.124	0.00	0.00
ARG118	HG2	1.00	2.127	0.00	0.00
ARG118	HG3	1.00	0.880	0.00	0.00
ARG118	HD2	1.00	0.002	1.00	0.23
ARG118	HD3	1.00	0.000	1.00	0.15
ARG118	HE	1.00	0.005	1.00	-1884892.00
ARG118	H	0.59	0.024	1.00	-697715.00

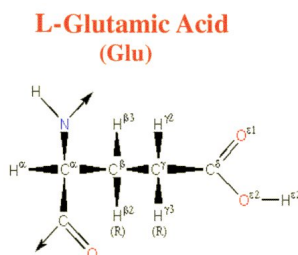


Figure 118: Image from the BMRB

Residue probability: 0.807
Residue probability confidence: 0.925

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	179.429	176.942	2.547	0.000	0.000
CA 3.119.1	59.530	57.442	3.837	0.600	1.000
CB 3.119.2	28.961	30.185	4.018	1.000	0.875
CG 3.119.3	36.010	36.085	1.533	0.886	0.875
N 3.119.4	122.419	120.574	4.837	0.841	1.000
HA 3.119.5	4.027	4.245	0.429	0.720	1.000
HB2 3.119.6	2.117	2.021	0.233	0.763	0.875
HB3 3.119.7	2.114	1.994	0.244	0.800	0.875
HG2 3.119.8	2.076	2.258	0.226	0.743	0.875
HG3 3.119.9	2.459	2.233	0.232	0.929	0.875
H 3.119.10	7.918	8.332	0.601	0.789	1.000
HE2	NA	—	—	0.000	0.000

3.119.1 Detailed Probabilities of GLU119CA:

Overall probability: 0.600
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG118	0.00	1.00
GLU119	0.67	1.00
PHE120	0.70	1.00

Expected NOESY Contacts

Proton	Expected probability
R118HA	1.00
E119HB2	1.00
E119HB3	1.00
E119HG2	1.00
E119HG3	1.00
E119H	1.00
E119HA	1.00
F120H	1.00
F120HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG118	HA	1.00	0.080	0.00	0.00
GLU119	HA	1.00	0.015	1.00	41.95
GLU119	HB2	1.00	0.039	0.10	0.00
GLU119	HB3	1.00	0.036	0.40	0.00
GLU119	HG2	1.00	0.002	1.00	5.05
GLU119	HG3	1.00	0.035	0.50	0.00
GLU119	H	1.00	0.006	1.00	0.81
PHE120	HA	1.00	0.020	1.00	41.95
PHE120	H	1.00	0.036	0.40	0.00

3.119.2 Detailed Probabilities of GLU119CB:

Overall probability: 1.000

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU119	1.00	0.86
PHE120	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E119HA	1.00
E119HB3	1.00
E119HG2	1.00
E119HG3	1.00
E119H	1.00
E119HE2	1.00
E119HB2	1.00
F120H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU119	HA	1.00	0.009	1.00	2.70
GLU119	HB2	1.00	0.024	1.00	35.26
GLU119	HB3	1.00	0.021	1.00	35.26
GLU119	HG2	1.00	0.017	1.00	35.26
GLU119	HG3	1.00	0.029	1.00	2.04
GLU119	H	1.00	0.018	1.00	1.51
PHE120	H	1.00	0.004	1.00	0.40
PHE120	HA	0.71	0.014	1.00	2.70

3.119.3 Detailed Probabilities of GLU119CG:

Overall probability: 0.886

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU119	0.87	0.86
PHE120	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E119HA	1.00
E119HB2	1.00
E119HB3	1.00
E119HG2	1.00
E119H	1.00
E119HE2	1.00
E119HG3	1.00
F120H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU119	HA	1.00	0.038	0.20	0.00
GLU119	HB2	1.00	0.026	1.00	3.11
GLU119	HB3	1.00	0.023	1.00	3.11
GLU119	HG2	1.00	0.010	1.00	6.84
GLU119	HG3	1.00	0.014	1.00	35.10
GLU119	H	1.00	0.006	1.00	0.43
PHE120	H	0.98	0.007	1.00	0.07

3.119.4 Detailed Probabilities of GLU119N:

Overall probability: 0.841

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG118	0.67	1.00
GLU119	0.93	1.00
PHE120	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R118HB3	1.00
R118HG2	0.98
R118H	1.00
R118HB2	1.00
R118HA	1.00
R118HG3	0.97
E119HA	1.00
E119HB2	1.00
E119HB3	1.00
E119HG2	1.00
E119HG3	1.00
E119H	1.00
F120H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG118	HA	1.00	0.003	1.00	-191191.00
ARG118	HB2	1.00	0.096	0.00	0.00
ARG118	HB3	1.00	0.024	1.00	-1423236.00
ARG118	HG2	0.98	0.118	0.02	0.00
ARG118	HG3	0.97	0.005	1.00	-114810.00
ARG118	H	1.00	0.003	1.00	-820448.00
GLU119	HA	1.00	0.001	1.00	-988122.00
GLU119	HB2	1.00	0.007	1.00	-2192989.00
GLU119	HB3	1.00	0.004	1.00	-2192989.00
GLU119	HG2	1.00	0.034	0.60	0.00
GLU119	HG3	1.00	0.002	1.00	-445241.00
GLU119	H	1.00	0.003	1.00	-9442289.00
PHE120	H	1.00	0.007	1.00	-694848.00
PHE120	HA	0.93	0.004	1.00	-988122.00
PHE120	HB2	0.59	0.028	1.00	-102209.00

3.119.5 Detailed Probabilities of GLU119HA:

Overall probability: 0.720

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG118	0.50	1.00
GLU119	0.87	1.00
PHE120	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
R118HA	1.00
E119HB2	1.00
E119HB3	1.00
E119HG2	1.00
E119HG3	1.00
E119H	1.00
E119HA	1.00
F120H	1.00
F120HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG118	HA	1.00	0.172	0.00	0.00
ARG118	HB3	0.79	0.015	1.00	0.54
GLU119	HA	1.00	0.015	1.00	41.95
GLU119	HB2	1.00	0.009	1.00	2.70
GLU119	HB3	1.00	0.009	1.00	2.70
GLU119	HG2	1.00	0.003	1.00	0.58
GLU119	HG3	1.00	0.038	0.20	0.00
GLU119	H	1.00	0.001	1.00	-988122.00
PHE120	HA	1.00	0.801	0.00	0.00
PHE120	H	1.00	0.002	1.00	-528983.00

3.119.6 Detailed Probabilities of GLU119HB2:

Overall probability: 0.763

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU119	0.68	0.86
PHE120	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E119HA	1.00
E119HB3	1.00
E119HG2	1.00
E119HG3	1.00
E119H	1.00
E119HE2	1.00
E119HB2	1.00
F120H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU119	HA	1.00	0.039	0.10	0.00
GLU119	HB2	1.00	0.024	1.00	35.26
GLU119	HB3	1.00	0.024	1.00	35.26
GLU119	HG2	1.00	0.339	0.00	0.00
GLU119	HG3	1.00	0.026	1.00	3.11
GLU119	H	1.00	0.007	1.00	-2192989.00
PHE120	H	1.00	0.007	1.00	-759428.00
PHE120	HA	0.71	0.011	1.00	0.12

3.119.7 Detailed Probabilities of GLU119HB3:

Overall probability: 0.800

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU119	0.73	0.86
PHE120	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E119HA	1.00
E119HB2	1.00
E119HG2	1.00
E119HG3	1.00
E119H	1.00
E119HE2	1.00
E119HB3	1.00
F120H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU119	HA	1.00	0.036	0.40	0.00
GLU119	HB2	1.00	0.021	1.00	35.26
GLU119	HB3	1.00	0.021	1.00	35.26
GLU119	HG2	1.00	0.342	0.00	0.00
GLU119	HG3	1.00	0.023	1.00	3.11
GLU119	H	1.00	0.004	1.00	-2192989.00
PHE120	H	1.00	0.004	1.00	-759428.00
PHE120	HA	0.85	0.008	1.00	0.12

3.119.8 Detailed Probabilities of GLU119HG2:

Overall probability: 0.743

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU119	0.77	0.86
PHE120	0.60	1.00

Expected NOESY Contacts

Proton	Expected probability
E119HA	1.00
E119HB2	1.00
E119HB3	1.00
E119HG3	1.00
E119H	1.00
E119HE2	1.00
E119HG2	1.00
F120H	0.99

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU119	HA	1.00	0.002	1.00	5.05
GLU119	HB2	1.00	0.017	1.00	35.26
GLU119	HB3	1.00	0.017	1.00	35.26
GLU119	HG2	1.00	0.337	0.00	0.00
GLU119	HG3	1.00	0.010	1.00	6.84
GLU119	H	1.00	0.034	0.60	0.00
PHE120	H	0.99	0.034	0.60	0.00

3.119.9 Detailed Probabilities of GLU119HG3:

Overall probability: 0.929

Overall confidence: 0.875

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU119	0.92	0.86
PHE120	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E119HA	1.00
E119HB2	1.00
E119HB3	1.00
E119HG2	1.00
E119H	1.00
E119HE2	1.00
E119HG3	1.00
F120H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU119	HA	1.00	0.035	0.50	0.00
GLU119	HB2	1.00	0.029	1.00	2.04
GLU119	HB3	1.00	0.029	1.00	2.04
GLU119	HG2	1.00	0.003	1.00	4.94
GLU119	HG3	1.00	0.014	1.00	35.10
GLU119	H	1.00	0.002	1.00	-445241.00
PHE120	H	0.98	0.008	1.00	-90717.00

3.119.10 Detailed Probabilities of GLU119H:

Overall probability: 0.789

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ARG118	0.58	1.00
GLU119	1.00	1.00
PHE120	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
R118HB3	1.00
R118HG2	0.98
R118H	1.00
R118HB2	1.00
R118HA	1.00
R118HG3	0.97
E119HA	1.00
E119HB2	1.00
E119HB3	1.00
E119HG2	1.00
E119HG3	1.00
E119H	1.00
F120H	1.00

NOESY contacts detailed probability

3.119 GLU(119)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ARG118	HA	1.00	0.005	1.00	0.30
ARG118	HB2	1.00	0.004	1.00	0.07
ARG118	HB3	1.00	0.005	1.00	0.17
ARG118	HG2	0.98	1.875	0.02	0.00
ARG118	HG3	0.97	0.628	0.03	0.00
ARG118	H	1.00	0.106	0.00	0.00
ARG118	HD2	0.58	0.003	1.00	0.06
GLU119	HA	1.00	0.006	1.00	0.81
GLU119	HB2	1.00	0.018	1.00	1.51
GLU119	HB3	1.00	0.018	1.00	1.51
GLU119	HG2	1.00	0.008	1.00	0.34
GLU119	HG3	1.00	0.006	1.00	0.43
GLU119	H	1.00	0.003	1.00	-9442289.00
PHE120	H	1.00	0.009	1.00	-615420.00

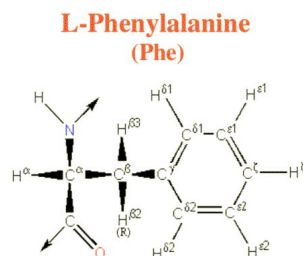


Figure 119: Image from the BMRB

Residue probability: 0.777
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	177.698	175.508	2.010	0.000	0.000
CA 3.120.1	56.868	58.245	3.808	0.667	1.000
CB 3.120.2	36.753	40.078	3.616	0.875	1.000
CD1 3.120.3	129.643	131.234	9.579	1.000	1.000
CD2 3.120.4	129.603	131.352	9.581	1.000	1.000
CE1 3.120.5	131.362	130.599	3.219	0.800	1.000
CE2 3.120.6	131.152	130.633	2.839	0.572	1.000
CZ 3.120.7	129.438	129.042	3.448	0.400	1.000
N 3.120.8	119.597	120.315	4.931	0.969	1.000
HA 3.120.9	4.022	4.625	1.237	0.667	1.000
HB2 3.120.10	3.218	2.980	0.399	0.875	1.000
HB3 3.120.11	2.343	2.916	0.434	0.625	1.000
HD1 3.120.12	6.789	7.037	0.347	1.000	1.000
HD2 3.120.13	6.789	7.022	0.417	1.000	1.000
HE1 3.120.14	7.137	7.046	0.417	0.833	1.000
HE2 3.120.15	7.137	7.043	0.400	0.572	1.000
HZ 3.120.16	7.019	6.984	1.598	0.400	1.000
H 3.120.17	8.826	8.375	0.710	0.954	1.000

3.120.1 Detailed Probabilities of PHE120CA:

Overall probability: 0.667
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU119	0.67	1.00
PHE120	0.86	1.00
MET121	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E119HA	1.00
F120HB2	1.00
F120HB3	1.00
F120HD1	1.00
F120HD2	1.00
F120H	1.00
F120HA	1.00
M121HA	1.00
M121H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU119	HA	1.00	0.801	0.00	0.00
GLU119	HB2	0.71	0.011	1.00	0.12
GLU119	HB3	0.85	0.008	1.00	0.12
PHE120	HA	1.00	0.796	0.00	0.00
PHE120	HB2	1.00	0.008	1.00	0.28
PHE120	HB3	1.00	0.001	1.00	0.32
PHE120	HD1	1.00	0.002	1.00	1.21
PHE120	HD2	1.00	0.002	1.00	1.21
PHE120	H	1.00	0.003	1.00	0.29
PHE120	HE1	0.74	0.007	1.00	0.16
MET121	HA	1.00	0.705	0.00	0.00
MET121	H	1.00	0.091	0.00	0.00

3.120.2 Detailed Probabilities of PHE120CB:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE120	0.86	1.00
MET121	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F120HA	1.00
F120HB3	1.00
F120HD1	1.00
F120HD2	1.00
F120HE2	1.00
F120H	1.00
F120HB2	1.00
M121H	1.00

NOESY contacts detailed probability

3.120 PHE(120)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE120	HA	1.00	0.001	1.00	0.17
PHE120	HB2	1.00	0.007	1.00	0.44
PHE120	HB3	1.00	0.005	1.00	0.46
PHE120	HD1	1.00	0.001	1.00	0.27
PHE120	HD2	1.00	0.001	1.00	0.27
PHE120	HE2	1.00	0.347	0.00	0.00
PHE120	H	1.00	0.003	1.00	0.16
MET121	H	1.00	0.007	1.00	0.12

3.120.3 Detailed Probabilities of PHE120CD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE120	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F120HA	1.00
F120HB2	1.00
F120HB3	1.00
F120HD2	1.00
F120HE1	1.00
F120HE2	1.00
F120HZ	1.00
F120H	1.00
F120HD1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE120	HA	1.00	0.006	1.00	1.59
PHE120	HB2	1.00	0.020	1.00	0.81
PHE120	HB3	1.00	0.006	1.00	0.54
PHE120	HD1	1.00	0.003	1.00	8.61
PHE120	HD2	1.00	0.003	1.00	8.61
PHE120	HE1	1.00	0.005	1.00	2.12
PHE120	HE2	1.00	0.005	1.00	2.12
PHE120	HZ	1.00	0.019	1.00	0.27
PHE120	H	1.00	0.007	1.00	0.35

3.120.4 Detailed Probabilities of PHE120CD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE120	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F120HA	1.00
F120HB2	1.00
F120HB3	1.00
F120HD1	1.00
F120HE1	1.00
F120HE2	1.00
F120HZ	1.00
F120H	0.99
F120HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE120	HA	1.00	0.006	1.00	1.59
PHE120	HB2	1.00	0.020	1.00	0.81
PHE120	HB3	1.00	0.006	1.00	0.54
PHE120	HD1	1.00	0.003	1.00	8.61
PHE120	HD2	1.00	0.003	1.00	8.61
PHE120	HE1	1.00	0.005	1.00	2.12
PHE120	HE2	1.00	0.005	1.00	2.12
PHE120	HZ	1.00	0.019	1.00	0.27
PHE120	H	0.99	0.007	1.00	0.35

3.120.5 Detailed Probabilities of PHE120CE1:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE120	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
F120HD1	1.00
F120HD2	1.00
F120HE2	1.00
F120HZ	1.00
F120HE1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE120	HD1	1.00	0.004	1.00	1.81
PHE120	HD2	1.00	0.004	1.00	1.81
PHE120	HE1	1.00	0.006	1.00	24.03
PHE120	HE2	1.00	0.006	1.00	24.03
PHE120	HZ	1.00	0.226	0.00	0.00

3.120.6 Detailed Probabilities of PHE120CE2:

Overall probability: 0.572

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE120	0.57	1.00

Expected NOESY Contacts

Proton	Expected probability
F120HB2	1.00
F120HB3	1.00
F120HD1	1.00
F120HD2	1.00
F120HE1	1.00
F120HZ	1.00
F120HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE120	HB2	1.00	0.943	0.00	0.00
PHE120	HB3	1.00	0.068	0.00	0.00
PHE120	HD1	1.00	0.004	1.00	1.81
PHE120	HD2	1.00	0.004	1.00	1.81
PHE120	HE1	1.00	0.006	1.00	24.03
PHE120	HE2	1.00	0.006	1.00	24.03
PHE120	HZ	1.00	0.124	0.00	0.00

3.120.7 Detailed Probabilities of PHE120CZ:

Overall probability: 0.400

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE120	0.40	1.00

Expected NOESY Contacts

Proton	Expected probability
F120HD1	1.00
F120HD2	1.00
F120HE1	1.00
F120HE2	1.00
F120HZ	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE120	HD1	1.00	0.013	1.00	0.27
PHE120	HD2	1.00	0.013	1.00	0.27
PHE120	HE1	1.00	0.335	0.00	0.00
PHE120	HE2	1.00	0.335	0.00	0.00
PHE120	HZ	1.00	0.217	0.00	0.00

3.120.8 Detailed Probabilities of PHE120N:

Overall probability: 0.969

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU119	0.93	1.00
PHE120	1.00	1.00
MET121	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E119HB3	1.00
E119HG3	0.98
E119HG2	0.99
E119HA	1.00
E119H	1.00
E119HB2	1.00
F120HA	1.00
F120HB2	1.00
F120HB3	1.00
F120HD1	1.00
F120HD2	0.99
F120H	1.00
M121H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU119	HA	1.00	0.002	1.00	-528983.00
GLU119	HB2	1.00	0.007	1.00	-759428.00
GLU119	HB3	1.00	0.004	1.00	-759428.00
GLU119	HG2	0.99	0.034	0.60	0.00
GLU119	HG3	0.98	0.008	1.00	-90717.00
GLU119	H	1.00	0.009	1.00	-615420.00
PHE120	HA	1.00	0.003	1.00	-528983.00
PHE120	HB2	1.00	0.015	1.00	-524127.00
PHE120	HB3	1.00	0.001	1.00	-300931.00
PHE120	HD1	1.00	0.002	1.00	-356902.00
PHE120	HD2	0.99	0.002	1.00	-356902.00
PHE120	H	1.00	0.002	1.00	-5590689.00
MET121	H	1.00	0.002	1.00	-348081.00

3.120.9 Detailed Probabilities of PHE120HA:

Overall probability: 0.667

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU119	1.00	1.00
PHE120	0.67	1.00
MET121	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E119HA	1.00
F120HB2	1.00
F120HB3	1.00
F120HD1	1.00
F120HD2	1.00
F120H	1.00
F120HA	1.00
M121HA	1.00
M121H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU119	HA	1.00	0.020	1.00	41.95
GLU119	HB2	0.71	0.014	1.00	2.70
GLU119	HB3	0.85	0.014	1.00	2.70
GLU119	H	0.93	0.004	1.00	-988122.00
PHE120	HA	1.00	0.796	0.00	0.00
PHE120	HB2	1.00	0.001	1.00	0.17
PHE120	HB3	1.00	0.220	0.00	0.00
PHE120	HD1	1.00	0.006	1.00	1.59
PHE120	HD2	1.00	0.006	1.00	1.59
PHE120	H	1.00	0.003	1.00	-528983.00
MET121	HA	1.00	0.764	0.00	0.00
MET121	H	1.00	0.080	0.00	0.00

3.120.10 Detailed Probabilities of PHE120HB2:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE120	0.86	1.00
MET121	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F120HA	1.00
F120HB3	1.00
F120HD1	1.00
F120HD2	1.00
F120HE2	1.00
F120H	1.00
F120HB2	1.00
M121H	1.00

NOESY contacts detailed probability

3.120 PHE(120)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE120	HA	1.00	0.008	1.00	0.28
PHE120	HB2	1.00	0.007	1.00	0.44
PHE120	HB3	1.00	0.006	1.00	0.51
PHE120	HD1	1.00	0.020	1.00	0.81
PHE120	HD2	1.00	0.020	1.00	0.81
PHE120	HE2	1.00	0.943	0.00	0.00
PHE120	H	1.00	0.015	1.00	-524127.00
MET121	H	1.00	0.011	1.00	-317943.00

3.120.11 Detailed Probabilities of PHE120HB3:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE120	0.71	1.00
MET121	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F120HA	1.00
F120HB2	1.00
F120HD1	1.00
F120HD2	1.00
F120HE2	1.00
F120H	1.00
F120HB3	1.00
M121H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE120	HA	1.00	0.001	1.00	0.32
PHE120	HB2	1.00	0.005	1.00	0.46
PHE120	HB3	1.00	0.205	0.00	0.00
PHE120	HD1	1.00	0.006	1.00	0.54
PHE120	HD2	1.00	0.006	1.00	0.54
PHE120	HE2	1.00	0.068	0.00	0.00
PHE120	H	1.00	0.001	1.00	-300931.00
MET121	H	1.00	0.054	0.00	0.00

3.120.12 Detailed Probabilities of PHE120HD1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE120	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F120HA	1.00
F120HB2	1.00
F120HB3	1.00
F120HD2	1.00
F120HE1	1.00
F120HE2	1.00
F120HZ	1.00
F120H	1.00
F120HD1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE120	HA	1.00	0.002	1.00	1.21
PHE120	HB2	1.00	0.001	1.00	0.27
PHE120	HB3	1.00	0.000	1.00	0.26
PHE120	HD1	1.00	0.003	1.00	8.61
PHE120	HD2	1.00	0.003	1.00	8.61
PHE120	HE1	1.00	0.004	1.00	1.81
PHE120	HE2	1.00	0.004	1.00	1.81
PHE120	HZ	1.00	0.013	1.00	0.27
PHE120	H	1.00	0.002	1.00	-356902.00

3.120.13 Detailed Probabilities of PHE120HD2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE120	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F120HA	1.00
F120HB2	1.00
F120HB3	1.00
F120HD1	1.00
F120HE1	1.00
F120HE2	1.00
F120HZ	1.00
F120H	0.99
F120HD2	1.00

NOESY contacts detailed probability

3.120 PHE(120)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE120	HA	1.00	0.002	1.00	1.21
PHE120	HB2	1.00	0.001	1.00	0.27
PHE120	HB3	1.00	0.000	1.00	0.26
PHE120	HD1	1.00	0.003	1.00	8.61
PHE120	HD2	1.00	0.003	1.00	8.61
PHE120	HE1	1.00	0.004	1.00	1.81
PHE120	HE2	1.00	0.004	1.00	1.81
PHE120	HZ	1.00	0.013	1.00	0.27
PHE120	H	0.99	0.002	1.00	-356902.00

3.120.14 Detailed Probabilities of PHE120HE1:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE120	0.83	1.00

Expected NOESY Contacts

Proton	Expected probability
F120HD1	1.00
F120HD2	1.00
F120HE2	1.00
F120HZ	1.00
F120HE1	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE120	HD1	1.00	0.005	1.00	2.12
PHE120	HD2	1.00	0.005	1.00	2.12
PHE120	HE1	1.00	0.006	1.00	24.03
PHE120	HE2	1.00	0.006	1.00	24.03
PHE120	HZ	1.00	0.335	0.00	0.00
PHE120	HA	0.74	0.007	1.00	0.16

3.120.15 Detailed Probabilities of PHE120HE2:

Overall probability: 0.572

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE120	0.57	1.00

Expected NOESY Contacts

Proton	Expected probability
F120HB2	1.00
F120HB3	1.00
F120HD1	1.00
F120HD2	1.00
F120HE1	1.00
F120HZ	1.00
F120HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE120	HB2	1.00	0.347	0.00	0.00
PHE120	HB3	1.00	0.348	0.00	0.00
PHE120	HD1	1.00	0.005	1.00	2.12
PHE120	HD2	1.00	0.005	1.00	2.12
PHE120	HE1	1.00	0.006	1.00	24.03
PHE120	HE2	1.00	0.006	1.00	24.03
PHE120	HZ	1.00	0.335	0.00	0.00

3.120.16 Detailed Probabilities of PHE120HZ:

Overall probability: 0.400

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE120	0.40	1.00

Expected NOESY Contacts

Proton	Expected probability
F120HD1	1.00
F120HD2	1.00
F120HE1	1.00
F120HE2	1.00
F120HZ	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE120	HD1	1.00	0.019	1.00	0.27
PHE120	HD2	1.00	0.019	1.00	0.27
PHE120	HE1	1.00	0.226	0.00	0.00
PHE120	HE2	1.00	0.124	0.00	0.00
PHE120	HZ	1.00	0.217	0.00	0.00

3.120.17 Detailed Probabilities of PHE120H:

Overall probability: 0.954

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU119	0.90	1.00
PHE120	1.00	1.00
MET121	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
E119HB3	1.00
E119HG3	0.98
E119HG2	0.99
E119HA	1.00
E119H	1.00
E119HB2	1.00
F120HA	1.00
F120HB2	1.00
F120HB3	1.00
F120HD1	1.00
F120HD2	0.99
F120H	1.00
M121H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU119	HA	1.00	0.036	0.40	0.00
GLU119	HB2	1.00	0.004	1.00	0.40
GLU119	HB3	1.00	0.004	1.00	0.40
GLU119	HG2	0.99	0.007	1.00	0.10
GLU119	HG3	0.98	0.007	1.00	0.07
GLU119	H	1.00	0.007	1.00	-694848.00
PHE120	HA	1.00	0.003	1.00	0.29
PHE120	HB2	1.00	0.003	1.00	0.16
PHE120	HB3	1.00	0.004	1.00	0.17
PHE120	HD1	1.00	0.007	1.00	0.35
PHE120	HD2	0.99	0.007	1.00	0.35
PHE120	H	1.00	0.002	1.00	-5590689.00
MET121	H	1.00	0.007	1.00	-422091.00

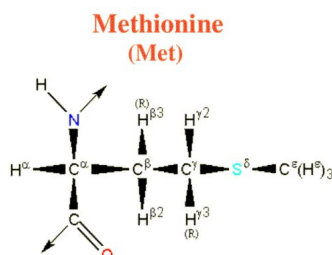
3.121 MET(121)

Figure 120: Image from the BMRB

Residue probability: 0.632

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	179.577	176.360	2.004	0.000	0.000
CA 3.121.1	59.785	56.303	4.222	0.178	1.000
CB 3.121.2	33.643	33.217	4.564	0.750	1.000
CG 3.121.3	31.222	32.123	4.122	0.692	1.000
CE 3.121.4	16.539	17.286	5.508	1.000	1.000
N 3.121.5	116.596	120.023	5.158	0.846	1.000
HA 3.121.6	3.931	4.409	0.504	0.600	1.000
HB2 3.121.7	2.290	2.016	0.340	0.625	1.000
HB3 3.121.8	2.077	1.978	0.359	0.563	1.000
HG2 3.121.9	1.917	2.410	0.360	0.513	1.000
HG3 3.121.10	2.625	2.378	0.386	0.829	1.000
HE 3.121.11	1.830	1.877	0.381	0.409	1.000
H 3.121.12	8.317	8.269	0.585	0.583	1.000

3.121.1 Detailed Probabilities of MET121CA:

Overall probability: 0.178

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE120	0.00	1.00
MET121	0.27	1.00
GLN122	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F120HA	1.00
M121HB2	1.00
M121HB3	1.00
M121HG2	1.00
M121HG3	1.00
M121H	1.00
M121HA	1.00
Q122H	1.00
Q122HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE120	HA	1.00	0.764	0.00	0.00
MET121	HA	1.00	0.855	0.00	0.00
MET121	HB2	1.00	0.108	0.00	0.00
MET121	HB3	1.00	0.007	1.00	0.44
MET121	HG2	1.00	0.153	0.00	0.00
MET121	HG3	1.00	0.034	0.60	0.00
MET121	H	1.00	0.090	0.00	0.00
GLN122	HA	1.00	0.651	0.00	0.00
GLN122	H	1.00	0.225	0.00	0.00

3.121.2 Detailed Probabilities of MET121CB:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET121	0.71	1.00
GLN122	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
M121HA	1.00
M121HB2	1.00
M121HG2	1.00
M121HG3	1.00
M121HE1	0.97
M121H	1.00
M121HB3	1.00
Q122H	1.00

NOESY contacts detailed probability

3.121 MET(121)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET121	HA	1.00	0.021	1.00	0.55
MET121	HB2	1.00	0.009	1.00	1.18
MET121	HB3	1.00	0.222	0.00	0.00
MET121	HG2	1.00	0.063	0.00	0.00
MET121	HG3	1.00	0.003	1.00	0.22
MET121	HE1	0.97	0.024	1.00	0.32
MET121	H	1.00	0.007	1.00	0.18
GLN122	H	1.00	0.004	1.00	0.15

3.121.3 Detailed Probabilities of MET121CG:

Overall probability: 0.692

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET121	0.79	1.00
GLN122	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
M121HA	1.00
M121HB2	1.00
M121HB3	1.00
M121HG2	1.00
M121HE1	1.00
M121H	1.00
M121HG3	1.00
Q122H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET121	HA	1.00	0.014	1.00	0.26
MET121	HB2	1.00	0.021	1.00	0.29
MET121	HB3	1.00	0.035	0.50	0.00
MET121	HG2	1.00	0.007	1.00	0.82
MET121	HG3	1.00	0.020	1.00	11.17
MET121	HE1	1.00	0.094	0.00	0.00
MET121	H	1.00	0.006	1.00	0.25
GLN122	H	0.97	0.269	0.03	0.00

3.121.4 Detailed Probabilities of MET121CE:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET121	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
M121HB2	0.96
M121HB3	0.97
M121HG2	1.00
M121HG3	1.00
M121HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET121	HB2	0.96	0.004	1.00	0.64
MET121	HB3	0.97	0.017	1.00	1.29
MET121	HG2	1.00	0.027	1.00	0.80
MET121	HG3	1.00	0.005	1.00	0.45
MET121	HE1	1.00	0.002	1.00	57.51

3.121.5 Detailed Probabilities of MET121N:

Overall probability: 0.846

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE120	0.67	1.00
MET121	1.00	1.00
GLN122	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F120HB2	1.00
F120HA	1.00
F120H	1.00
F120HB3	1.00
M121HA	1.00
M121HB2	1.00
M121HB3	1.00
M121HG2	1.00
M121HG3	1.00
M121H	1.00
Q122H	1.00

NOESY contacts detailed probability

3.121 MET(121)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE120	HA	1.00	0.080	0.00	0.00
PHE120	HB2	1.00	0.011	1.00	-317943.00
PHE120	HB3	1.00	0.054	0.00	0.00
PHE120	H	1.00	0.007	1.00	-422091.00
PHE120	HD1	0.83	0.001	1.00	-146143.00
PHE120	HD2	0.71	0.001	1.00	-146143.00
MET121	HA	1.00	0.011	1.00	-426602.00
MET121	HB2	1.00	0.001	1.00	-534760.00
MET121	HB3	1.00	0.001	1.00	-382872.00
MET121	HG2	1.00	0.006	1.00	-378787.00
MET121	HG3	1.00	0.002	1.00	-482988.00
MET121	H	1.00	0.005	1.00	-3547864.00
GLN122	H	1.00	0.001	1.00	-637644.00

3.121.6 Detailed Probabilities of MET121HA:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE120	0.00	1.00
MET121	0.71	1.00
GLN122	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
F120HA	1.00
M121HB2	1.00
M121HB3	1.00
M121HG2	1.00
M121HG3	1.00
M121H	1.00
M121HA	1.00
Q122H	1.00
Q122HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE120	HA	1.00	0.705	0.00	0.00
MET121	HA	1.00	0.855	0.00	0.00
MET121	HB2	1.00	0.000	1.00	0.25
MET121	HB3	1.00	0.021	1.00	0.55
MET121	HG2	1.00	1.300	0.00	0.00
MET121	HG3	1.00	0.014	1.00	0.26
MET121	H	1.00	0.011	1.00	-426602.00
MET121	HE1	0.69	0.030	1.00	0.00
GLN122	HA	1.00	0.115	0.00	0.00
GLN122	H	1.00	0.001	1.00	-172528.00

3.121.7 Detailed Probabilities of MET121HB2:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET121	0.71	1.00
GLN122	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
M121HA	1.00
M121HB3	1.00
M121HG2	1.00
M121HG3	1.00
M121HE1	0.96
M121H	1.00
M121HB2	1.00
Q122H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET121	HA	1.00	0.108	0.00	0.00
MET121	HB2	1.00	0.000	1.00	4.69
MET121	HB3	1.00	0.009	1.00	1.18
MET121	HG2	1.00	0.225	0.00	0.00
MET121	HG3	1.00	0.021	1.00	0.29
MET121	HE1	0.96	0.004	1.00	0.64
MET121	H	1.00	0.001	1.00	-534760.00
GLN122	H	1.00	0.043	0.00	0.00

3.121.8 Detailed Probabilities of MET121HB3:

Overall probability: 0.563

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET121	0.50	1.00
GLN122	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
M121HA	1.00
M121HB2	1.00
M121HG2	1.00
M121HG3	1.00
M121HE1	0.97
M121H	1.00
M121HB3	1.00
Q122H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET121	HA	1.00	0.007	1.00	0.44
MET121	HB2	1.00	0.121	0.00	0.00
MET121	HB3	1.00	0.222	0.00	0.00
MET121	HG2	1.00	0.438	0.00	0.00
MET121	HG3	1.00	0.035	0.50	0.00
MET121	HE1	0.97	0.017	1.00	1.29
MET121	H	1.00	0.001	1.00	-382872.00
GLN122	H	1.00	0.005	1.00	-335811.00

3.121.9 Detailed Probabilities of MET121HG2:

Overall probability: 0.513

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET121	0.44	1.00
GLN122	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
M121HA	1.00
M121HB2	1.00
M121HB3	1.00
M121HG3	1.00
M121HE1	1.00
M121H	1.00
M121HG2	1.00
Q122H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET121	HA	1.00	0.153	0.00	0.00
MET121	HB2	1.00	0.039	0.10	0.00
MET121	HB3	1.00	0.063	0.00	0.00
MET121	HG2	1.00	0.598	0.00	0.00
MET121	HG3	1.00	0.007	1.00	0.82
MET121	HE1	1.00	0.027	1.00	0.80
MET121	H	1.00	0.006	1.00	-378787.00
GLN122	H	0.98	0.006	1.00	-202086.00

3.121.10 Detailed Probabilities of MET121HG3:

Overall probability: 0.829

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET121	0.94	1.00
GLN122	0.03	1.00

Expected NOESY Contacts

Proton	Expected probability
M121HA	1.00
M121HB2	1.00
M121HB3	1.00
M121HG2	1.00
M121HE1	1.00
M121H	1.00
M121HG3	1.00
Q122H	0.97

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET121	HA	1.00	0.034	0.60	0.00
MET121	HB2	1.00	0.006	1.00	0.18
MET121	HB3	1.00	0.003	1.00	0.22
MET121	HG2	1.00	0.006	1.00	0.86
MET121	HG3	1.00	0.020	1.00	11.17
MET121	HE1	1.00	0.005	1.00	0.45
MET121	H	1.00	0.002	1.00	-482988.00
GLN122	H	0.97	0.102	0.03	0.00

3.121.11 Detailed Probabilities of MET121HE1:

Overall probability: 0.409

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET121	0.41	1.00

Expected NOESY Contacts

Proton	Expected probability
M121HB2	0.96
M121HB3	0.97
M121HG2	1.00
M121HG3	1.00
M121HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET121	HB2	0.96	0.105	0.04	0.00
MET121	HB3	0.97	0.024	1.00	0.32
MET121	HG2	1.00	0.685	0.00	0.00
MET121	HG3	1.00	0.094	0.00	0.00
MET121	HE1	1.00	0.002	1.00	57.51

3.121.12 Detailed Probabilities of MET121H:

Overall probability: 0.583

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
PHE120	0.50	1.00
MET121	0.50	1.00
GLN122	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
F120HB2	1.00
F120HA	1.00
F120H	1.00
F120HB3	1.00
M121HA	1.00
M121HB2	1.00
M121HB3	1.00
M121HG2	1.00
M121HG3	1.00
M121H	1.00
Q122H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
PHE120	HA	1.00	0.091	0.00	0.00
PHE120	HB2	1.00	0.007	1.00	0.12
PHE120	HB3	1.00	0.155	0.00	0.00
PHE120	H	1.00	0.002	1.00	-348081.00
MET121	HA	1.00	0.090	0.00	0.00
MET121	HB2	1.00	0.264	0.00	0.00
MET121	HB3	1.00	0.007	1.00	0.18
MET121	HG2	1.00	1.538	0.00	0.00
MET121	HG3	1.00	0.006	1.00	0.25
MET121	H	1.00	0.005	1.00	-3547864.00
GLN122	H	1.00	0.010	1.00	-572584.00
GLN122	HA	0.89	0.009	1.00	0.12



Figure 121: Image from the BMRB

Residue probability: 0.772
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	178.893	176.405	1.998	0.000	0.000
CA 3.122.1	58.745	56.667	2.318	0.667	1.000
CB 3.122.2	28.020	29.436	2.799	0.556	1.000
CG 3.122.3	33.526	33.781	1.871	1.000	1.000
N 3.122.4	120.565	119.799	3.762	0.860	1.000
NE2 3.122.5	111.549	111.924	2.434	1.000	1.000
HA 3.122.6	4.135	4.265	0.455	0.750	1.000
HB 3.122.7	2.241	2.047	0.290	0.625	1.000
HG2 3.122.8	2.406	2.308	0.289	0.875	1.000
HG3 3.122.9	2.521	2.284	0.313	0.755	1.000
H 3.122.10	8.054	8.232	0.711	0.773	1.000
HE21 3.122.11	7.466	7.217	0.496	0.800	1.000
HE22 3.122.12	6.831	7.041	0.463	0.600	1.000

3.122.1 Detailed Probabilities of GLN122CA:

Overall probability: 0.667
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET121	0.50	1.00
GLN122	1.00	1.00
LYS123	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
M121HA	1.00
Q122HB2	1.00
Q122HG2	1.00
Q122HG3	1.00
Q122H	1.00
Q122HA	1.00
K123HA	1.00
K123H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET121	HA	1.00	0.115	0.00	0.00
MET121	H	0.89	0.009	1.00	0.12
GLN122	HA	1.00	0.010	1.00	24.81
GLN122	HB2	1.00	0.008	1.00	2.15
GLN122	HG2	1.00	0.006	1.00	0.81
GLN122	HG3	1.00	0.007	1.00	0.35
GLN122	H	1.00	0.008	1.00	1.25
LYS123	HA	1.00	0.120	0.00	0.00
LYS123	H	1.00	0.040	0.00	0.00

3.122.2 Detailed Probabilities of GLN122CB:

Overall probability: 0.556

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN122	0.43	1.00
LYS123	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q122HA	1.00
Q122HB3	1.00
Q122HG2	1.00
Q122HG3	1.00
Q122H	1.00
Q122HE21	1.00
Q122HE22	1.00
K123H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN122	HA	1.00	0.010	1.00	1.11
GLN122	HB2	1.00	0.006	1.00	9.16
GLN122	HG2	1.00	0.159	0.00	0.00
GLN122	HG3	1.00	0.274	0.00	0.00
GLN122	H	1.00	0.004	1.00	1.07
GLN122	HE21	1.00	0.592	0.00	0.00
GLN122	HE22	1.00	1.227	0.00	0.00
LYS123	H	1.00	0.010	1.00	0.51
LYS123	HA	0.82	0.006	1.00	0.56

3.122.3 Detailed Probabilities of GLN122CG:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN122	1.00	1.00
LYS123	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q122HA	1.00
Q122HB2	1.00
Q122HG2	1.00
Q122H	1.00
Q122HE21	1.00
Q122HE22	1.00
Q122HG3	1.00
K123H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN122	HA	1.00	0.008	1.00	0.75
GLN122	HB2	1.00	0.008	1.00	2.01
GLN122	HG2	1.00	0.000	1.00	10.45
GLN122	HG3	1.00	0.003	1.00	28.96
GLN122	H	1.00	0.003	1.00	0.45
GLN122	HE21	1.00	0.002	1.00	0.15
GLN122	HE22	1.00	0.006	1.00	0.14
LYS123	H	0.96	0.004	1.00	0.13

3.122.4 Detailed Probabilities of GLN122N:

Overall probability: 0.860

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET121	0.67	1.00
GLN122	1.00	1.00
LYS123	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
M121HB3	1.00
M121H	1.00
M121HA	1.00
M121HB2	1.00
M121HG2	0.98
M121HG3	0.97
Q122HA	1.00
Q122HB2	1.00
Q122HG2	1.00
Q122HG3	1.00
Q122H	1.00
K123H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET121	HA	1.00	0.001	1.00	-172528.00
MET121	HB2	1.00	0.043	0.00	0.00
MET121	HB3	1.00	0.005	1.00	-335811.00
MET121	HG2	0.98	0.006	1.00	-202086.00
MET121	HG3	0.97	0.102	0.03	0.00
MET121	H	1.00	0.010	1.00	-572584.00
GLN122	HA	1.00	0.010	1.00	-859418.00
GLN122	HB2	1.00	0.006	1.00	-1820309.00
GLN122	HG2	1.00	0.006	1.00	-423662.00
GLN122	HG3	1.00	0.002	1.00	-351425.00
GLN122	H	1.00	0.004	1.00	-7514558.00
LYS123	H	1.00	0.007	1.00	-820512.00
LYS123	HA	0.87	0.002	1.00	-413103.00
LYS123	HB2	0.56	0.011	1.00	-202086.00

3.122.5 Detailed Probabilities of GLN122NE2:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN122	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q122HB2	1.00
Q122HG2	1.00
Q122HG3	1.00
Q122HE22	1.00
Q122HE21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN122	HB2	1.00	0.009	1.00	-86167.00
GLN122	HG2	1.00	0.001	1.00	-139457.00
GLN122	HG3	1.00	0.005	1.00	-227687.00
GLN122	HE21	1.00	0.001	1.00	-27659210.00
GLN122	HE22	1.00	0.001	1.00	-14655499.00

3.122.6 Detailed Probabilities of GLN122HA:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET121	0.00	1.00
GLN122	1.00	1.00
LYS123	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
M121HA	1.00
Q122HB2	1.00
Q122HG2	1.00
Q122HG3	1.00
Q122H	1.00
Q122HA	1.00
K123HA	1.00
K123H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET121	HA	1.00	0.651	0.00	0.00
GLN122	HA	1.00	0.010	1.00	24.81
GLN122	HB2	1.00	0.010	1.00	1.11
GLN122	HG2	1.00	0.001	1.00	1.02
GLN122	HG3	1.00	0.008	1.00	0.75
GLN122	H	1.00	0.010	1.00	-859418.00
LYS123	HA	1.00	0.093	0.00	0.00
LYS123	H	1.00	0.010	1.00	-702515.00

3.122.7 Detailed Probabilities of GLN122HB2:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN122	0.71	1.00
LYS123	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q122HA	1.00
Q122HB3	1.00
Q122HG2	1.00
Q122HG3	1.00
Q122H	1.00
Q122HE21	1.00
Q122HE22	1.00
K123H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN122	HA	1.00	0.008	1.00	2.15
GLN122	HB2	1.00	0.006	1.00	9.16
GLN122	HG2	1.00	0.051	0.00	0.00
GLN122	HG3	1.00	0.008	1.00	2.01
GLN122	H	1.00	0.006	1.00	-1820309.00
GLN122	HE21	1.00	0.009	1.00	-86167.00
GLN122	HE22	1.00	0.170	0.00	0.00
LYS123	H	1.00	0.156	0.00	0.00

3.122.8 Detailed Probabilities of GLN122HG2:

Overall probability: 0.875

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN122	0.86	1.00
LYS123	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q122HA	1.00
Q122HB2	1.00
Q122HG3	1.00
Q122H	1.00
Q122HE21	1.00
Q122HE22	1.00
Q122HG2	1.00
K123H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN122	HA	1.00	0.006	1.00	0.81
GLN122	HB2	1.00	0.159	0.00	0.00
GLN122	HG2	1.00	0.010	1.00	103.18
GLN122	HG3	1.00	0.000	1.00	10.45
GLN122	H	1.00	0.006	1.00	-423662.00
GLN122	HE21	1.00	0.001	1.00	-139457.00
GLN122	HE22	1.00	0.005	1.00	-120738.00
LYS123	H	0.98	0.009	1.00	-173082.00

3.122.9 Detailed Probabilities of GLN122HG3:

Overall probability: 0.755

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN122	0.86	1.00
LYS123	0.04	1.00

Expected NOESY Contacts

Proton	Expected probability
Q122HA	1.00
Q122HB2	1.00
Q122HG2	1.00
Q122H	1.00
Q122HE21	1.00
Q122HE22	1.00
Q122HG3	1.00
K123H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN122	HA	1.00	0.007	1.00	0.35
GLN122	HB2	1.00	0.274	0.00	0.00
GLN122	HG2	1.00	0.005	1.00	10.18
GLN122	HG3	1.00	0.003	1.00	28.96
GLN122	H	1.00	0.002	1.00	-351425.00
GLN122	HE21	1.00	0.005	1.00	-227687.00
GLN122	HE22	1.00	0.002	1.00	-130588.00
LYS123	H	0.96	0.052	0.04	0.00

3.122.10 Detailed Probabilities of GLN122H:

Overall probability: 0.773

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
MET121	0.51	1.00
GLN122	1.00	1.00
LYS123	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
M121HB3	1.00
M121H	1.00
M121HA	1.00
M121HB2	1.00
M121HG2	0.98
M121HG3	0.97
Q122HA	1.00
Q122HB2	1.00
Q122HG2	1.00
Q122HG3	1.00
Q122H	1.00
K123H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
MET121	HA	1.00	0.225	0.00	0.00
MET121	HB2	1.00	0.001	1.00	0.15
MET121	HB3	1.00	0.004	1.00	0.15
MET121	HG2	0.98	1.456	0.02	0.00
MET121	HG3	0.97	0.269	0.03	0.00
MET121	H	1.00	0.001	1.00	-637644.00
GLN122	HA	1.00	0.008	1.00	1.25
GLN122	HB2	1.00	0.004	1.00	1.07
GLN122	HG2	1.00	0.003	1.00	0.50
GLN122	HG3	1.00	0.003	1.00	0.45
GLN122	H	1.00	0.004	1.00	-7514558.00
LYS123	H	1.00	0.007	1.00	-701537.00
LYS123	HB2	0.56	0.023	1.00	1.13

3.122.11 Detailed Probabilities of GLN122HE21:

Overall probability: 0.800

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN122	0.80	1.00

Expected NOESY Contacts

Proton	Expected probability
Q122HB2	1.00
Q122HG2	1.00
Q122HG3	1.00
Q122HE22	1.00
Q122HE21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN122	HB2	1.00	0.592	0.00	0.00
GLN122	HG2	1.00	0.014	1.00	0.20
GLN122	HG3	1.00	0.002	1.00	0.15
GLN122	HE21	1.00	0.001	1.00	-27659210.00
GLN122	HE22	1.00	0.001	1.00	-14177617.00

3.122.12 Detailed Probabilities of GLN122HE22:

Overall probability: 0.600

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN122	0.60	1.00

Expected NOESY Contacts

Proton	Expected probability
Q122HB2	1.00
Q122HG2	1.00
Q122HG3	1.00
Q122HE21	1.00
Q122HE22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN122	HB2	1.00	1.227	0.00	0.00
GLN122	HG2	1.00	0.065	0.00	0.00
GLN122	HG3	1.00	0.006	1.00	0.14
GLN122	HE21	1.00	0.001	1.00	-14655499.00
GLN122	HE22	1.00	0.001	1.00	-36164948.00

Proton	Expected probability
Q122HA	1.00
K123HB2	1.00
K123HB3	1.00
K123HG2	1.00
K123HG3	1.00
K123HD2	0.98
K123HD3	0.98
K123H	1.00
K123HA	1.00
A124H	1.00
A124HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN122	HA	1.00	0.093	0.00	0.00
LYS123	HA	1.00	0.017	1.00	41.95
LYS123	HB2	1.00	0.007	1.00	3.48
LYS123	HB3	1.00	0.027	1.00	3.48
LYS123	HG2	1.00	0.111	0.00	0.00
LYS123	HG3	1.00	0.012	1.00	1.91
LYS123	HD2	0.98	0.157	0.02	0.00
LYS123	HD3	0.98	0.062	0.02	0.00
LYS123	H	1.00	0.000	1.00	0.35
ALA124	HA	1.00	0.102	0.00	0.00
ALA124	H	1.00	0.005	1.00	0.37

3.123.2 Detailed Probabilities of LYS123CB:

Overall probability: 0.639

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS123	0.60	1.00
ALA124	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K123HA	1.00
K123HB3	1.00
K123HG2	1.00
K123HG3	1.00
K123HD2	1.00
K123HD3	1.00
K123HE2	0.98
K123HE3	0.99
K123H	1.00
K123HB2	1.00
A124H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS123	HA	1.00	0.204	0.00	0.00
LYS123	HB2	1.00	0.030	1.00	0.00
LYS123	HB3	1.00	0.010	1.00	53.87
LYS123	HG2	1.00	0.008	1.00	3.20
LYS123	HG3	1.00	0.015	1.00	5.56
LYS123	HD2	1.00	0.160	0.00	0.00
LYS123	HD3	1.00	0.017	1.00	5.01
LYS123	HE2	0.98	0.084	0.02	0.00
LYS123	HE3	0.99	0.080	0.01	0.00
LYS123	H	1.00	0.010	1.00	0.44
ALA124	H	1.00	0.008	1.00	0.34

3.123.3 Detailed Probabilities of LYS123CG:

Overall probability: 0.740

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS123	0.81	0.91
ALA124	0.04	1.00

Expected NOESY Contacts

Proton	Expected probability
K123HA	1.00
K123HB2	1.00
K123HB3	1.00
K123HG2	1.00
K123HD2	1.00
K123HD3	1.00
K123HE2	1.00
K123HE3	1.00
K123H	1.00
K123HZ2	1.00
K123HG3	1.00
A124H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS123	HA	1.00	0.010	1.00	0.26
LYS123	HB2	1.00	0.004	1.00	1.27
LYS123	HB3	1.00	0.024	1.00	1.27
LYS123	HG2	1.00	0.007	1.00	3.14
LYS123	HG3	1.00	0.011	1.00	11.48
LYS123	HD2	1.00	0.095	0.00	0.00
LYS123	HD3	1.00	0.039	0.10	0.00
LYS123	HE2	1.00	0.005	1.00	0.55
LYS123	HE3	1.00	0.001	1.00	0.55
LYS123	H	1.00	0.007	1.00	0.33
ALA124	H	0.96	0.194	0.04	0.00

3.123.4 Detailed Probabilities of LYS123CD:

Overall probability: 0.420

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS123	0.42	0.90

Expected NOESY Contacts

Proton	Expected probability
K123HA	0.98
K123HB2	1.00
K123HB3	1.00
K123HG2	1.00
K123HG3	1.00
K123HD3	1.00
K123HE2	1.00
K123HE3	1.00
K123HZ2	1.00
K123HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS123	HA	0.98	0.001	1.00	0.18
LYS123	HB2	1.00	0.196	0.00	0.00
LYS123	HB3	1.00	0.176	0.00	0.00
LYS123	HG2	1.00	0.163	0.00	0.00
LYS123	HG3	1.00	0.040	0.00	0.00
LYS123	HD2	1.00	0.105	0.00	0.00
LYS123	HD3	1.00	0.010	1.00	4.77
LYS123	HE2	1.00	0.032	0.80	0.00
LYS123	HE3	1.00	0.036	0.40	0.00
LYS123	H	0.88	0.012	1.00	0.09

3.123.5 Detailed Probabilities of LYS123CE:

Overall probability: 0.875

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS123	0.88	0.89

Expected NOESY Contacts

Proton	Expected probability
K123HB2	0.98
K123HB3	0.99
K123HG2	1.00
K123HG3	1.00
K123HD2	1.00
K123HD3	1.00
K123HE3	1.00
K123HZ2	1.00
K123HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS123	HB2	0.98	0.021	1.00	0.39
LYS123	HB3	0.99	0.016	1.00	1.41
LYS123	HG2	1.00	0.008	1.00	1.46
LYS123	HG3	1.00	0.002	1.00	15.02
LYS123	HD2	1.00	0.009	1.00	1.17
LYS123	HD3	1.00	0.052	0.00	0.00
LYS123	HE2	1.00	0.017	1.00	227.40
LYS123	HE3	1.00	0.021	1.00	227.40

3.123.6 Detailed Probabilities of LYS123N:

Overall probability: 0.626

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN122	0.61	1.00
LYS123	0.68	1.00
ALA124	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
Q122HG2	0.98
Q122HA	1.00
Q122HB3	1.00
Q122H	1.00
Q122HG3	0.96
K123HA	1.00
K123HB2	1.00
K123HB3	1.00
K123HG2	1.00
K123HG3	1.00
K123H	1.00
A124H	1.00

NOESY contacts detailed probability

3.123 LYS(123)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN122	HA	1.00	0.010	1.00	-702515.00
GLN122	HB2	1.00	0.156	0.00	0.00
GLN122	HG2	0.98	0.009	1.00	-173082.00
GLN122	HG3	0.96	0.052	0.04	0.00
GLN122	H	1.00	0.007	1.00	-701537.00
LYS123	HA	1.00	0.008	1.00	-317410.00
LYS123	HB2	1.00	0.013	1.00	-855024.00
LYS123	HB3	1.00	0.007	1.00	-855024.00
LYS123	HG2	1.00	0.065	0.00	0.00
LYS123	HG3	1.00	0.039	0.10	0.00
LYS123	H	1.00	0.017	1.00	-9420832.00
ALA124	H	1.00	0.218	0.00	0.00
ALA124	HA	0.90	0.019	1.00	-702515.00

3.123.7 Detailed Probabilities of LYS123HA:

Overall probability: 0.463

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN122	0.67	1.00
LYS123	0.50	1.00
ALA124	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q122HA	1.00
K123HB2	1.00
K123HB3	1.00
K123HG2	1.00
K123HG3	1.00
K123HD2	0.98
K123HD3	0.98
K123H	1.00
K123HA	1.00
A124H	1.00
A124HA	1.00

NOESY contacts detailed probability

3.123 LYS(123)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN122	HA	1.00	0.120	0.00	0.00
GLN122	HB2	0.68	0.006	1.00	0.56
GLN122	H	0.87	0.002	1.00	-413103.00
LYS123	HA	1.00	0.017	1.00	41.95
LYS123	HB2	1.00	0.204	0.00	0.00
LYS123	HB3	1.00	0.060	0.00	0.00
LYS123	HG2	1.00	0.981	0.00	0.00
LYS123	HG3	1.00	0.010	1.00	0.26
LYS123	HD2	0.98	0.001	1.00	0.18
LYS123	HD3	0.98	0.647	0.02	0.00
LYS123	H	1.00	0.008	1.00	-317410.00
ALA124	HA	1.00	0.119	0.00	0.00
ALA124	H	1.00	0.068	0.00	0.00

3.123.8 Detailed Probabilities of LYS123HB2:

Overall probability: 0.727

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS123	0.70	1.00
ALA124	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K123HA	1.00
K123HB3	1.00
K123HG2	1.00
K123HG3	1.00
K123HD2	1.00
K123HD3	1.00
K123HE2	0.98
K123HE3	0.99
K123H	1.00
K123HB2	1.00
A124H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS123	HA	1.00	0.007	1.00	3.48
LYS123	HB2	1.00	0.030	1.00	0.00
LYS123	HB3	1.00	0.030	1.00	0.00
LYS123	HG2	1.00	0.894	0.00	0.00
LYS123	HG3	1.00	0.004	1.00	1.27
LYS123	HD2	1.00	0.196	0.00	0.00
LYS123	HD3	1.00	0.094	0.00	0.00
LYS123	HE2	0.98	0.021	1.00	0.39
LYS123	HE3	0.99	0.004	1.00	1.41
LYS123	H	1.00	0.013	1.00	-855024.00
ALA124	H	1.00	0.010	1.00	-530958.00

3.123.9 Detailed Probabilities of LYS123HB3:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS123	0.70	1.00
ALA124	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K123HA	1.00
K123HB2	1.00
K123HG2	1.00
K123HG3	1.00
K123HD2	1.00
K123HD3	1.00
K123HE2	0.99
K123HE3	0.99
K123H	1.00
K123HB3	1.00
A124H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS123	HA	1.00	0.027	1.00	3.48
LYS123	HB2	1.00	0.010	1.00	53.87
LYS123	HB3	1.00	0.010	1.00	53.87
LYS123	HG2	1.00	0.874	0.00	0.00
LYS123	HG3	1.00	0.024	1.00	1.27
LYS123	HD2	1.00	0.176	0.00	0.00
LYS123	HD3	1.00	0.074	0.00	0.00
LYS123	HE2	0.99	0.016	1.00	1.41
LYS123	HE3	0.99	0.016	1.00	1.41
LYS123	H	1.00	0.007	1.00	-855024.00
ALA124	H	1.00	0.010	1.00	-530958.00
ALA124	HA	0.84	0.015	1.00	0.34

3.123.10 Detailed Probabilities of LYS123HG2:

Overall probability: 0.545

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS123	0.50	0.91
ALA124	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K123HA	1.00
K123HB2	1.00
K123HB3	1.00
K123HG3	1.00
K123HD2	1.00
K123HD3	1.00
K123HE2	1.00
K123HE3	1.00
K123H	1.00
K123HZ2	1.00
K123HG2	1.00
A124H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS123	HA	1.00	0.111	0.00	0.00
LYS123	HB2	1.00	0.008	1.00	3.20
LYS123	HB3	1.00	0.008	1.00	3.20
LYS123	HG2	1.00	0.535	0.00	0.00
LYS123	HG3	1.00	0.007	1.00	3.14
LYS123	HD2	1.00	0.163	0.00	0.00
LYS123	HD3	1.00	0.265	0.00	0.00
LYS123	HE2	1.00	0.008	1.00	1.46
LYS123	HE3	1.00	0.012	1.00	2.64
LYS123	H	1.00	0.065	0.00	0.00
ALA124	H	0.98	0.018	1.00	-96504.00

3.123.11 Detailed Probabilities of LYS123HG3:

Overall probability: 0.645

Overall confidence: 0.917

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS123	0.61	0.91
ALA124	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K123HA	1.00
K123HB2	1.00
K123HB3	1.00
K123HG2	1.00
K123HD2	1.00
K123HD3	1.00
K123HE2	1.00
K123HE3	1.00
K123H	1.00
K123HZ2	1.00
K123HG3	1.00
A124H	0.96

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS123	HA	1.00	0.012	1.00	1.91
LYS123	HB2	1.00	0.015	1.00	5.56
LYS123	HB3	1.00	0.015	1.00	5.56
LYS123	HG2	1.00	0.658	0.00	0.00
LYS123	HG3	1.00	0.011	1.00	11.48
LYS123	HD2	1.00	0.040	0.00	0.00
LYS123	HD3	1.00	0.142	0.00	0.00
LYS123	HE2	1.00	0.002	1.00	15.02
LYS123	HE3	1.00	0.002	1.00	15.02
LYS123	H	1.00	0.039	0.10	0.00
ALA124	H	0.96	0.013	1.00	-107012.00

3.123.12 Detailed Probabilities of LYS123HD2:

Overall probability: 0.335

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS123	0.34	0.90

Expected NOESY Contacts

Proton	Expected probability
K123HA	0.98
K123HB2	1.00
K123HB3	1.00
K123HG2	1.00
K123HG3	1.00
K123HD3	1.00
K123HE2	1.00
K123HE3	1.00
K123HZ2	1.00
K123HD2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS123	HA	0.98	0.157	0.02	0.00
LYS123	HB2	1.00	0.160	0.00	0.00
LYS123	HB3	1.00	0.061	0.00	0.00
LYS123	HG2	1.00	0.803	0.00	0.00
LYS123	HG3	1.00	0.095	0.00	0.00
LYS123	HD2	1.00	0.105	0.00	0.00
LYS123	HD3	1.00	0.003	1.00	4.53
LYS123	HE2	1.00	0.009	1.00	1.17
LYS123	HE3	1.00	0.009	1.00	1.17

3.123.13 Detailed Probabilities of LYS123HD3:

Overall probability: 0.347

Overall confidence: 0.900

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS123	0.35	0.90

Expected NOESY Contacts

Proton	Expected probability
K123HA	0.98
K123HB2	1.00
K123HB3	1.00
K123HG2	1.00
K123HG3	1.00
K123HD2	1.00
K123HE2	1.00
K123HE3	1.00
K123HZ2	1.00
K123HD3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS123	HA	0.98	0.062	0.02	0.00
LYS123	HB2	1.00	0.017	1.00	5.01
LYS123	HB3	1.00	0.017	1.00	5.01
LYS123	HG2	1.00	0.708	0.00	0.00
LYS123	HG3	1.00	0.039	0.10	0.00
LYS123	HD2	1.00	0.010	1.00	4.77
LYS123	HD3	1.00	0.092	0.00	0.00
LYS123	HE2	1.00	0.052	0.00	0.00
LYS123	HE3	1.00	0.052	0.00	0.00

3.123.14 Detailed Probabilities of LYS123HE2:

Overall probability: 0.591

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS123	0.59	0.89

Expected NOESY Contacts

Proton	Expected probability
K123HB2	0.98
K123HB3	0.99
K123HG2	1.00
K123HG3	1.00
K123HD2	1.00
K123HD3	1.00
K123HE3	1.00
K123HZ2	1.00
K123HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS123	HB2	0.98	0.084	0.02	0.00
LYS123	HB3	0.99	0.084	0.01	0.00
LYS123	HG2	1.00	0.031	0.90	0.00
LYS123	HG3	1.00	0.005	1.00	0.55
LYS123	HD2	1.00	0.032	0.80	0.00
LYS123	HD3	1.00	0.176	0.00	0.00
LYS123	HE2	1.00	0.017	1.00	227.40
LYS123	HE3	1.00	0.026	1.00	641.65

3.123.15 Detailed Probabilities of LYS123HE3:

Overall probability: 0.491

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS123	0.49	0.89

Expected NOESY Contacts

Proton	Expected probability
K123HB2	0.99
K123HB3	0.99
K123HG2	1.00
K123HG3	1.00
K123HD2	1.00
K123HD3	1.00
K123HE2	1.00
K123HZ2	1.00
K123HE3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS123	HB2	0.99	0.080	0.01	0.00
LYS123	HB3	0.99	0.080	0.01	0.00
LYS123	HG2	1.00	0.035	0.50	0.00
LYS123	HG3	1.00	0.001	1.00	0.55
LYS123	HD2	1.00	0.036	0.40	0.00
LYS123	HD3	1.00	0.180	0.00	0.00
LYS123	HE2	1.00	0.021	1.00	227.40
LYS123	HE3	1.00	0.022	1.00	641.65

3.123.16 Detailed Probabilities of LYS123H:

Overall probability: 0.887

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
GLN122	0.66	1.00
LYS123	1.00	1.00
ALA124	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
Q122HG2	0.98
Q122HA	1.00
Q122HB3	1.00
Q122H	1.00
Q122HG3	0.96
K123HA	1.00
K123HB2	1.00
K123HB3	1.00
K123HG2	1.00
K123HG3	1.00
K123H	1.00
A124H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLN122	HA	1.00	0.040	0.00	0.00
GLN122	HB2	1.00	0.010	1.00	0.51
GLN122	HG2	0.98	0.037	0.30	0.00
GLN122	HG3	0.96	0.004	1.00	0.13
GLN122	H	1.00	0.007	1.00	-820512.00
LYS123	HA	1.00	0.000	1.00	0.35
LYS123	HB2	1.00	0.010	1.00	0.44
LYS123	HB3	1.00	0.010	1.00	0.44
LYS123	HG2	1.00	0.009	1.00	0.25
LYS123	HG3	1.00	0.007	1.00	0.33
LYS123	H	1.00	0.017	1.00	-9420832.00
LYS123	HD2	0.88	0.012	1.00	0.09
LYS123	HD3	0.87	0.014	1.00	0.11
ALA124	H	1.00	0.009	1.00	-618975.00
ALA124	HA	0.90	0.023	1.00	0.06

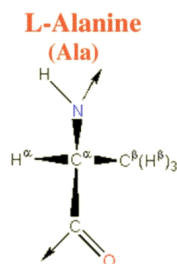
3.124 ALA(124)

Figure 123: Image from the BMRB

Residue probability: 0.821

Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
CA 3.124.1	54.652	53.289	3.425	0.565	1.000
CB 3.124.2	18.934	19.355	4.103	1.000	1.000
N 3.124.3	121.873	123.100	4.487	0.900	1.000
HA 3.124.4	4.144	4.254	0.459	0.625	1.000
HB 3.124.5	1.504	1.346	0.258	1.000	1.000
H 3.124.6	8.601	8.206	0.601	0.837	1.000

3.124.1 Detailed Probabilities of ALA124CA:

Overall probability: 0.565

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS123	0.66	1.00
ALA124	1.00	1.00
GLY125	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K123HA	1.00
A124H	1.00
A124HB1	1.00
A124HA	1.00
G125HA3	1.00
G125H	1.00
G125HA2	1.00

NOESY contacts detailed probability

3.124 ALA(124)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS123	HA	1.00	0.119	0.00	0.00
LYS123	HB2	0.65	0.035	0.65	0.00
LYS123	HB3	0.84	0.015	1.00	0.34
LYS123	H	0.90	0.023	1.00	0.06
ALA124	HA	1.00	0.000	1.00	9.26
ALA124	HB1	1.00	0.001	1.00	1.82
ALA124	H	1.00	0.007	1.00	0.55
GLY125	HA2	1.00	0.092	0.00	0.00
GLY125	HA3	1.00	0.081	0.00	0.00
GLY125	H	1.00	0.058	0.00	0.00

3.124.2 Detailed Probabilities of ALA124CB:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ALA124	1.00	1.00
GLY125	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
A124HA	1.00
A124H	1.00
A124HB2	1.00
G125H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA124	HA	1.00	0.000	1.00	2.09
ALA124	HB1	1.00	0.001	1.00	30.14
ALA124	H	1.00	0.006	1.00	1.39
GLY125	H	1.00	0.003	1.00	0.44

3.124.3 Detailed Probabilities of ALA124N:

Overall probability: 0.900

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS123	0.83	1.00
ALA124	1.00	1.00
GLY125	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K123H	1.00
K123HG3	0.96
K123HB3	1.00
K123HB2	1.00
K123HG2	0.98
K123HA	1.00
A124HA	1.00
A124HB1	1.00
A124H	1.00
G125H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS123	HA	1.00	0.068	0.00	0.00
LYS123	HB2	1.00	0.010	1.00	-530958.00
LYS123	HB3	1.00	0.010	1.00	-530958.00
LYS123	HG2	0.98	0.018	1.00	-96504.00
LYS123	HG3	0.96	0.013	1.00	-107012.00
LYS123	H	1.00	0.009	1.00	-618975.00
ALA124	HA	1.00	0.006	1.00	-846356.00
ALA124	HB1	1.00	0.000	1.00	-1567496.00
ALA124	H	1.00	0.004	1.00	-6488405.00
GLY125	H	1.00	0.006	1.00	-487040.00

3.124.4 Detailed Probabilities of ALA124HA:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS123	0.50	1.00
ALA124	1.00	1.00
GLY125	0.33	1.00

Expected NOESY Contacts

Proton	Expected probability
K123HA	1.00
A124H	1.00
A124HB1	1.00
A124HA	1.00
G125HA3	1.00
G125H	1.00
G125HA2	1.00

NOESY contacts detailed probability

3.124 ALA(124)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS123	HA	1.00	0.102	0.00	0.00
LYS123	H	0.90	0.019	1.00	-702515.00
ALA124	HA	1.00	0.000	1.00	9.26
ALA124	HB1	1.00	0.000	1.00	2.09
ALA124	H	1.00	0.006	1.00	-846356.00
GLY125	HA2	1.00	0.094	0.00	0.00
GLY125	HA3	1.00	0.094	0.00	0.00
GLY125	H	1.00	0.010	1.00	-478065.00

3.124.5 Detailed Probabilities of ALA124HB1:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ALA124	1.00	1.00
GLY125	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
A124HA	1.00
A124H	1.00
A124HB2	1.00
G125H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA124	HA	1.00	0.001	1.00	1.82
ALA124	HB1	1.00	0.001	1.00	30.14
ALA124	H	1.00	0.000	1.00	-1567496.00
GLY125	H	1.00	0.001	1.00	-636121.00
GLY125	HA2	0.56	0.004	1.00	0.18
GLY125	HA3	0.60	0.004	1.00	0.18

3.124.6 Detailed Probabilities of ALA124H:

Overall probability: 0.837

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LYS123	0.67	1.00
ALA124	1.00	1.00
GLY125	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
K123H	1.00
K123HG3	0.96
K123HB3	1.00
K123HB2	1.00
K123HG2	0.98
K123HA	1.00
A124HA	1.00
A124HB1	1.00
A124H	1.00
G125H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LYS123	HA	1.00	0.005	1.00	0.37
LYS123	HB2	1.00	0.008	1.00	0.34
LYS123	HB3	1.00	0.008	1.00	0.34
LYS123	HG2	0.98	0.007	1.00	0.06
LYS123	HG3	0.96	0.194	0.04	0.00
LYS123	H	1.00	0.218	0.00	0.00
ALA124	HA	1.00	0.007	1.00	0.55
ALA124	HB1	1.00	0.006	1.00	1.39
ALA124	H	1.00	0.004	1.00	-6488405.00
GLY125	H	1.00	0.006	1.00	-498794.00
GLY125	HA2	0.71	0.006	1.00	0.07
GLY125	HA3	0.75	0.006	1.00	0.07

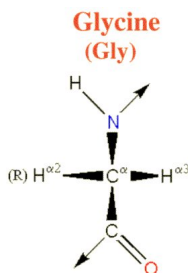


Figure 124: Image from the BMRB

Residue probability: 0.844
Residue probability confidence: 1.000

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	175.553	173.872	2.493	0.000	0.000
CA 3.125.1	46.291	45.581	4.381	0.778	1.000
N 3.125.2	104.755	109.752	5.331	1.000	1.000
HA2 3.125.3	4.052	3.967	0.380	0.857	1.000
HA3 3.125.4	4.063	3.897	0.390	0.833	1.000
H 3.125.5	7.949	8.343	0.939	0.750	1.000

3.125.1 Detailed Probabilities of GLY125CA:

Overall probability: 0.778
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ALA124	0.67	1.00
GLY125	1.00	1.00
SER126	0.67	1.00

Expected NOESY Contacts

Proton	Expected probability
A124HA	1.00
G125HA3	1.00
G125H	1.00
G125HA2	1.00
S126HA	1.00
S126H	1.00

NOESY contacts detailed probability

3.125 GLY(125)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA124	HA	1.00	0.094	0.00	0.00
ALA124	HB1	0.53	0.004	1.00	0.18
ALA124	H	0.71	0.006	1.00	0.07
GLY125	HA2	1.00	0.002	1.00	6.79
GLY125	HA3	1.00	0.013	1.00	6.79
GLY125	H	1.00	0.007	1.00	1.04
SER126	HA	1.00	0.020	1.00	0.09
SER126	H	1.00	0.095	0.00	0.00
SER126	HB2	0.59	0.027	1.00	6.79

3.125.2 Detailed Probabilities of GLY125N:

Overall probability: 1.000

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ALA124	1.00	1.00
GLY125	1.00	1.00
SER126	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
A124HB1	1.00
A124H	1.00
A124HA	1.00
G125HA2	1.00
G125HA3	1.00
G125H	1.00
S126H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA124	HA	1.00	0.010	1.00	-478065.00
ALA124	HB1	1.00	0.001	1.00	-636121.00
ALA124	H	1.00	0.006	1.00	-498794.00
GLY125	HA2	1.00	0.003	1.00	-1613012.00
GLY125	HA3	1.00	0.014	1.00	-1613012.00
GLY125	H	1.00	0.009	1.00	-4557853.00
SER126	H	1.00	0.014	1.00	-418606.00

3.125.3 Detailed Probabilities of GLY125HA2:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ALA124	0.00	1.00
GLY125	1.00	1.00
SER126	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
A124HA	1.00
G125HA3	1.00
G125H	1.00
G125HA2	1.00
S126HA	1.00
S126H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA124	HA	1.00	0.092	0.00	0.00
GLY125	HA2	1.00	0.002	1.00	6.79
GLY125	HA3	1.00	0.002	1.00	6.79
GLY125	H	1.00	0.003	1.00	-1613012.00
SER126	HA	1.00	0.019	1.00	1.99
SER126	H	1.00	0.016	1.00	-1734742.00
SER126	HB2	0.59	0.021	1.00	30.82

3.125.4 Detailed Probabilities of GLY125HA3:

Overall probability: 0.833

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ALA124	0.00	1.00
GLY125	1.00	1.00
SER126	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
A124HA	1.00
G125HA2	1.00
G125H	1.00
G125HA3	1.00
S126HA	1.00
S126H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA124	HA	1.00	0.081	0.00	0.00
GLY125	HA2	1.00	0.013	1.00	6.79
GLY125	HA3	1.00	0.013	1.00	6.79
GLY125	H	1.00	0.014	1.00	-1613012.00
SER126	HA	1.00	0.030	1.00	1.99
SER126	H	1.00	0.027	1.00	-1734742.00

3.125.5 Detailed Probabilities of GLY125H:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
ALA124	0.67	1.00
GLY125	1.00	1.00
SER126	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
A124HB1	1.00
A124H	1.00
A124HA	1.00
G125HA2	1.00
G125HA3	1.00
G125H	1.00
S126H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
ALA124	HA	1.00	0.058	0.00	0.00
ALA124	HB1	1.00	0.003	1.00	0.44
ALA124	H	1.00	0.006	1.00	-487040.00
GLY125	HA2	1.00	0.007	1.00	1.04
GLY125	HA3	1.00	0.007	1.00	1.04
GLY125	H	1.00	0.009	1.00	-4557853.00
SER126	H	1.00	0.082	0.00	0.00
SER126	HA	0.86	0.012	1.00	0.10

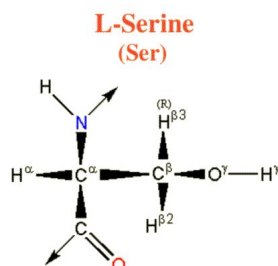


Figure 125: Image from the BMRB

Residue probability: 0.890
Residue probability confidence: 0.865

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	175.504	174.682	1.868	0.000	0.000
CA 3.126.1	59.965	58.750	3.025	0.911	0.889
CB 3.126.2	63.460	63.523	4.288	1.000	0.833
N 3.126.3	116.080	116.135	5.326	0.889	0.889
HA 3.126.4	4.447	4.486	0.430	1.000	0.889
HB2 3.126.5	4.023	3.856	0.325	0.833	0.833
HB3 3.126.6	4.030	3.825	0.343	0.833	0.833
H 3.126.7	7.861	8.292	0.600	0.767	0.889
HG	NA	—	—	0.000	0.000

3.126.1 Detailed Probabilities of SER126CA:

Overall probability: 0.911
Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
GLY125	1.00	1.00
SER126	1.00	0.80
LEU127	0.60	1.00

Expected NOESY Contacts

Proton	Expected probability
G125HA3	1.00
G125HA2	1.00
S126HB2	1.00
S126HB3	1.00
S126H	1.00
S126HG	1.00
S126HA	1.00
L127H	1.00
L127HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLY125	HA2	1.00	0.019	1.00	1.99
GLY125	HA3	1.00	0.030	1.00	1.99
GLY125	H	0.86	0.012	1.00	0.10
SER126	HA	1.00	0.007	1.00	9.89
SER126	HB2	1.00	0.010	1.00	1.99
SER126	HB3	1.00	0.003	1.00	1.99
SER126	H	1.00	0.019	1.00	0.65
LEU127	HA	1.00	0.038	0.20	0.00
LEU127	H	1.00	0.002	1.00	0.65

3.126.2 Detailed Probabilities of SER126CB:

Overall probability: 1.000

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
SER126	1.00	0.80
LEU127	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S126HA	1.00
S126HB3	1.00
S126H	1.00
S126HG	1.00
S126HB2	1.00
L127H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER126	HA	1.00	0.006	1.00	2.16
SER126	HB2	1.00	0.008	1.00	30.82
SER126	HB3	1.00	0.001	1.00	30.82
SER126	H	1.00	0.013	1.00	1.09
LEU127	H	1.00	0.008	1.00	1.09

3.126.3 Detailed Probabilities of SER126N:

Overall probability: 0.889

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
GLY125	0.67	1.00
SER126	1.00	0.80
LEU127	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
G125HA3	1.00
G125H	1.00
G125HA2	1.00
S126HA	1.00
S126HB2	1.00
S126HB3	1.00
S126HG	1.00
S126H	1.00
L127H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLY125	HA2	1.00	0.016	1.00	-1734742.00
GLY125	HA3	1.00	0.027	1.00	-1734742.00
GLY125	H	1.00	0.082	0.00	0.00
SER126	HA	1.00	0.007	1.00	-643287.00
SER126	HB2	1.00	0.013	1.00	-1734742.00
SER126	HB3	1.00	0.006	1.00	-1734742.00
SER126	H	1.00	0.006	1.00	-5223082.00
LEU127	H	1.00	0.015	1.00	-5223082.00
LEU127	HB2	0.57	0.028	1.00	-124842.00

3.126.4 Detailed Probabilities of SER126HA:

Overall probability: 1.000

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
GLY125	1.00	1.00
SER126	1.00	0.80
LEU127	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
G125HA3	1.00
G125HA2	1.00
S126HB2	1.00
S126HB3	1.00
S126H	1.00
S126HG	1.00
S126HA	1.00
L127H	1.00
L127HA	1.00

NOESY contacts detailed probability

3.126 SER(126)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLY125	HA2	1.00	0.020	1.00	0.09
GLY125	HA3	1.00	0.020	1.00	0.09
SER126	HA	1.00	0.007	1.00	9.89
SER126	HB2	1.00	0.006	1.00	2.16
SER126	HB3	1.00	0.006	1.00	2.16
SER126	H	1.00	0.007	1.00	-643287.00
LEU127	HA	1.00	0.005	1.00	0.21
LEU127	H	1.00	0.007	1.00	-476980.00

3.126.5 Detailed Probabilities of SER126HB2:

Overall probability: 0.833

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
SER126	1.00	0.80
LEU127	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
S126HA	1.00
S126HB3	1.00
S126H	1.00
S126HG	1.00
S126HB2	1.00
L127H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER126	HA	1.00	0.010	1.00	1.99
SER126	HB2	1.00	0.008	1.00	30.82
SER126	HB3	1.00	0.008	1.00	30.82
SER126	H	1.00	0.013	1.00	-1734742.00
LEU127	H	1.00	0.122	0.00	0.00
LEU127	HA	0.68	0.016	1.00	0.06

3.126.6 Detailed Probabilities of SER126HB3:

Overall probability: 0.833

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
SER126	1.00	0.80
LEU127	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
S126HA	1.00
S126HB2	1.00
S126H	1.00
S126HG	1.00
S126HB3	1.00
L127H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER126	HA	1.00	0.003	1.00	1.99
SER126	HB2	1.00	0.001	1.00	30.82
SER126	HB3	1.00	0.001	1.00	30.82
SER126	H	1.00	0.006	1.00	-1734742.00
LEU127	H	1.00	0.115	0.00	0.00
LEU127	HA	0.76	0.023	1.00	0.06

3.126.7 Detailed Probabilities of SER126H:

Overall probability: 0.767

Overall confidence: 0.889

Inter- and intra-residue probability

Residue	Probability	Confidence
GLY125	0.33	1.00
SER126	1.00	0.80
LEU127	0.95	1.00

Expected NOESY Contacts

Proton	Expected probability
G125HA3	1.00
G125H	1.00
G125HA2	1.00
S126HA	1.00
S126HB2	1.00
S126HB3	1.00
S126HG	1.00
S126H	1.00
L127H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLY125	HA2	1.00	0.095	0.00	0.00
GLY125	HA3	1.00	0.095	0.00	0.00
GLY125	H	1.00	0.014	1.00	-418606.00
SER126	HA	1.00	0.019	1.00	0.65
SER126	HB2	1.00	0.013	1.00	1.09
SER126	HB3	1.00	0.013	1.00	1.09
SER126	H	1.00	0.006	1.00	-5223082.00
LEU127	H	1.00	0.031	0.90	0.00
LEU127	HB2	0.57	0.027	1.00	0.51

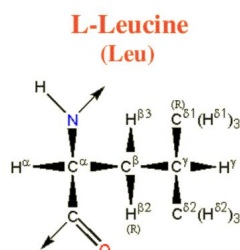


Figure 126: Image from the BMRB

Residue probability: 0.702
Residue probability confidence: 0.986

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	177.990	177.056	1.929	0.000	0.000
CA 3.127.1	56.217	55.735	3.802	0.567	1.000
CB 3.127.2	42.073	42.389	3.750	0.750	1.000
CG 3.127.3	26.770	26.892	3.086	0.503	1.000
CD1 3.127.4	25.524	24.837	3.657	0.714	1.000
CD2 3.127.5	22.960	24.201	3.117	0.857	1.000
N 3.127.6	122.372	121.785	4.943	0.723	0.909
HA 3.127.7	4.282	4.315	0.840	0.820	1.000
HB2 3.127.8	1.933	1.601	0.373	0.625	1.000
HB3 3.127.9	1.613	1.508	0.398	0.889	1.000
HG 3.127.10	1.858	1.510	0.340	0.413	1.000
HD1 3.127.11	1.012	0.739	0.294	0.715	1.000
HD2 3.127.12	0.931	0.727	0.421	0.714	1.000
H 3.127.13	7.882	8.237	0.647	0.833	0.909

3.127.1 Detailed Probabilities of LEU127CA:

Overall probability: 0.567
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
SER126	1.00	1.00
LEU127	0.40	1.00
GLU128	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
S126HA	1.00
L127HB2	1.00
L127HB3	1.00
L127HG	1.00
L127HD11	0.99
L127HD21	0.99
L127H	1.00
L127HA	1.00
E128HA	1.00
E128H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER126	HA	1.00	0.005	1.00	0.21
SER126	HB2	0.68	0.016	1.00	0.06
SER126	HB3	0.76	0.023	1.00	0.06
LEU127	HA	1.00	0.028	1.00	21.81
LEU127	HB2	1.00	0.032	0.80	0.00
LEU127	HB3	1.00	0.546	0.00	0.00
LEU127	HG	1.00	0.791	0.00	0.00
LEU127	HD11	0.99	0.055	0.01	0.00
LEU127	HD21	0.99	0.008	1.00	1.93
LEU127	H	1.00	0.089	0.00	0.00
GLU128	HA	1.00	0.814	0.00	0.00
GLU128	H	1.00	0.003	1.00	0.42

3.127.2 Detailed Probabilities of LEU127CB:

Overall probability: 0.750

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU127	0.86	1.00
GLU128	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L127HA	1.00
L127HB2	1.00
L127HG	1.00
L127HD11	1.00
L127HD21	1.00
L127H	1.00
L127HB3	1.00
E128H	1.00

NOESY contacts detailed probability

3.127 LEU(127)

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Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU127	HA	1.00	0.006	1.00	0.85
LEU127	HB2	1.00	0.001	1.00	3.52
LEU127	HB3	1.00	0.025	1.00	8.63
LEU127	HG	1.00	0.074	0.00	0.00
LEU127	HD11	1.00	0.009	1.00	0.91
LEU127	HD21	1.00	0.020	1.00	1.80
LEU127	H	1.00	0.008	1.00	0.44
GLU128	H	1.00	0.164	0.00	0.00

3.127.3 Detailed Probabilities of LEU127CG:

Overall probability: 0.503

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU127	0.57	1.00
GLU128	0.02	1.00

Expected NOESY Contacts

Proton	Expected probability
L127HA	1.00
L127HB2	1.00
L127HB3	1.00
L127HD11	1.00
L127HD21	1.00
L127H	1.00
L127HG	1.00
E128H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU127	HA	1.00	0.002	1.00	0.36
LEU127	HB2	1.00	0.062	0.00	0.00
LEU127	HB3	1.00	0.018	1.00	0.88
LEU127	HG	1.00	0.013	1.00	12.24
LEU127	HD11	1.00	0.249	0.00	0.00
LEU127	HD21	1.00	0.196	0.00	0.00
LEU127	H	1.00	0.006	1.00	0.59
GLU128	H	0.98	0.080	0.02	0.00

3.127.4 Detailed Probabilities of LEU127CD1:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU127	0.71	1.00

Expected NOESY Contacts

Proton	Expected probability
L127HA	0.99
L127HB2	1.00
L127HB3	1.00
L127HG	1.00
L127HD12	1.00
L127HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU127	HA	0.99	0.001	1.00	0.22
LEU127	HB2	1.00	0.012	1.00	1.05
LEU127	HB3	1.00	0.001	1.00	1.12
LEU127	HG	1.00	0.063	0.00	0.00
LEU127	HD11	1.00	0.003	1.00	54.17
LEU127	HD21	1.00	0.084	0.00	0.00
LEU127	H	0.86	0.010	1.00	0.11

3.127.5 Detailed Probabilities of LEU127CD2:

Overall probability: 0.857

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU127	0.86	1.00

Expected NOESY Contacts

Proton	Expected probability
L127HA	0.99
L127HB2	1.00
L127HB3	1.00
L127HG	1.00
L127HD11	1.00
L127HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU127	HA	0.99	0.006	1.00	1.72
LEU127	HB2	1.00	0.084	0.00	0.00
LEU127	HB3	1.00	0.006	1.00	1.03
LEU127	HG	1.00	0.009	1.00	2.84
LEU127	HD11	1.00	0.021	1.00	1.09
LEU127	HD21	1.00	0.001	1.00	78.89
LEU127	H	0.85	0.005	1.00	0.06

3.127.6 Detailed Probabilities of LEU127N:

Overall probability: 0.723

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
SER126	0.47	0.80
LEU127	0.79	1.00
GLU128	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S126HG	0.97
S126HB3	1.00
S126H	1.00
S126HB2	1.00
S126HA	1.00
L127HA	1.00
L127HB2	1.00
L127HB3	1.00
L127HG	1.00
L127H	1.00
E128H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER126	HA	1.00	0.007	1.00	-476980.00
SER126	HB2	1.00	0.122	0.00	0.00
SER126	HB3	1.00	0.115	0.00	0.00
SER126	H	1.00	0.031	0.90	0.00
LEU127	HA	1.00	0.006	1.00	-684269.00
LEU127	HB2	1.00	0.038	0.20	0.00
LEU127	HB3	1.00	0.002	1.00	-634901.00
LEU127	HG	1.00	0.037	0.30	0.00
LEU127	H	1.00	0.010	1.00	-9319551.00
LEU127	HD11	0.88	0.021	1.00	-380039.00
LEU127	HD21	0.87	0.025	1.00	-389307.00
GLU128	H	1.00	0.002	1.00	-703601.00
GLU128	HB2	0.55	0.006	1.00	-1423236.00

3.127.7 Detailed Probabilities of LEU127HA:

Overall probability: 0.820

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
SER126	0.20	1.00
LEU127	1.00	1.00
GLU128	0.50	1.00

Expected NOESY Contacts

Proton	Expected probability
S126HA	1.00
L127HB2	1.00
L127HB3	1.00
L127HG	1.00
L127HD11	0.99
L127HD21	0.99
L127H	1.00
L127HA	1.00
E128HA	1.00
E128H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER126	HA	1.00	0.038	0.20	0.00
LEU127	HA	1.00	0.028	1.00	21.81
LEU127	HB2	1.00	0.003	1.00	0.49
LEU127	HB3	1.00	0.006	1.00	0.85
LEU127	HG	1.00	0.002	1.00	0.36
LEU127	HD11	0.99	0.001	1.00	0.22
LEU127	HD21	0.99	0.006	1.00	1.72
LEU127	H	1.00	0.006	1.00	-684269.00
GLU128	HA	1.00	0.007	1.00	0.07
GLU128	H	1.00	0.059	0.00	0.00

3.127.8 Detailed Probabilities of LEU127HB2:

Overall probability: 0.625

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU127	0.57	1.00
GLU128	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L127HA	1.00
L127HB3	1.00
L127HG	1.00
L127HD11	1.00
L127HD21	1.00
L127H	1.00
L127HB2	1.00
E128H	1.00

NOESY contacts detailed probability

3.127 LEU(127)

Areca @ NMRFAM

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU127	HA	1.00	0.032	0.80	0.00
LEU127	HB2	1.00	0.007	1.00	5.90
LEU127	HB3	1.00	0.001	1.00	3.52
LEU127	HG	1.00	0.062	0.00	0.00
LEU127	HD11	1.00	0.012	1.00	1.05
LEU127	HD21	1.00	0.084	0.00	0.00
LEU127	H	1.00	0.038	0.20	0.00
GLU128	H	1.00	0.017	1.00	-1585593.00

3.127.9 Detailed Probabilities of LEU127HB3:

Overall probability: 0.889

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU127	0.86	1.00
GLU128	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L127HA	1.00
L127HB2	1.00
L127HG	1.00
L127HD11	1.00
L127HD21	1.00
L127H	1.00
L127HB3	1.00
E128H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU127	HA	1.00	0.546	0.00	0.00
LEU127	HB2	1.00	0.015	1.00	3.74
LEU127	HB3	1.00	0.025	1.00	8.63
LEU127	HG	1.00	0.018	1.00	0.88
LEU127	HD11	1.00	0.001	1.00	1.12
LEU127	HD21	1.00	0.006	1.00	1.03
LEU127	H	1.00	0.002	1.00	-634901.00
GLU128	H	1.00	0.018	1.00	-892233.00
GLU128	HA	0.90	0.024	1.00	0.71

3.127.10 Detailed Probabilities of LEU127HG:

Overall probability: 0.413

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU127	0.33	1.00
GLU128	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L127HA	1.00
L127HB2	1.00
L127HB3	1.00
L127HD11	1.00
L127HD21	1.00
L127H	1.00
L127HG	1.00
E128H	0.98

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU127	HA	1.00	0.791	0.00	0.00
LEU127	HB2	1.00	0.068	0.00	0.00
LEU127	HB3	1.00	0.074	0.00	0.00
LEU127	HG	1.00	0.013	1.00	12.24
LEU127	HD11	1.00	0.063	0.00	0.00
LEU127	HD21	1.00	0.009	1.00	2.84
LEU127	H	1.00	0.037	0.30	0.00
GLU128	H	0.98	0.002	1.00	-207979.00

3.127.11 Detailed Probabilities of LEU127HD11:

Overall probability: 0.715

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU127	0.72	1.00

Expected NOESY Contacts

Proton	Expected probability
L127HA	0.99
L127HB2	1.00
L127HB3	1.00
L127HG	1.00
L127HD12	1.00
L127HD21	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU127	HA	0.99	0.055	0.01	0.00
LEU127	HB2	1.00	0.000	1.00	0.78
LEU127	HB3	1.00	0.009	1.00	0.91
LEU127	HG	1.00	0.249	0.00	0.00
LEU127	HD11	1.00	0.003	1.00	54.17
LEU127	HD21	1.00	0.021	1.00	1.09
LEU127	H	0.86	0.021	1.00	-380039.00

3.127.12 Detailed Probabilities of LEU127HD21:

Overall probability: 0.714

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU127	0.71	1.00

Expected NOESY Contacts

Proton	Expected probability
L127HA	0.99
L127HB2	1.00
L127HB3	1.00
L127HG	1.00
L127HD11	1.00
L127HD22	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU127	HA	0.99	0.008	1.00	1.93
LEU127	HB2	1.00	0.017	1.00	1.66
LEU127	HB3	1.00	0.020	1.00	1.80
LEU127	HG	1.00	0.196	0.00	0.00
LEU127	HD11	1.00	0.084	0.00	0.00
LEU127	HD21	1.00	0.001	1.00	78.89
LEU127	H	0.85	0.025	1.00	-389307.00

3.127.13 Detailed Probabilities of LEU127H:

Overall probability: 0.833

Overall confidence: 0.909

Inter- and intra-residue probability

Residue	Probability	Confidence
SER126	1.00	0.80
LEU127	0.86	1.00
GLU128	0.00	1.00

Expected NOESY Contacts

Proton	Expected probability
S126HG	0.97
S126HB3	1.00
S126H	1.00
S126HB2	1.00
S126HA	1.00
L127HA	1.00
L127HB2	1.00
L127HB3	1.00
L127HG	1.00
L127H	1.00
E128H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
SER126	HA	1.00	0.002	1.00	0.65
SER126	HB2	1.00	0.008	1.00	1.09
SER126	HB3	1.00	0.008	1.00	1.09
SER126	H	1.00	0.015	1.00	-5223082.00
LEU127	HA	1.00	0.089	0.00	0.00
LEU127	HB2	1.00	0.006	1.00	0.51
LEU127	HB3	1.00	0.008	1.00	0.44
LEU127	HG	1.00	0.006	1.00	0.59
LEU127	H	1.00	0.010	1.00	-9319551.00
LEU127	HD11	0.88	0.010	1.00	0.11
LEU127	HD21	0.87	0.005	1.00	0.06
GLU128	H	1.00	0.064	0.00	0.00

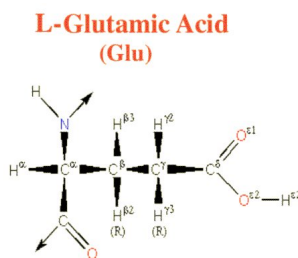


Figure 127: Image from the BMRB

Residue probability: 0.620
Residue probability confidence: 0.907

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	NA	—	—	0.000	0.000
CA 3.128.1	57.611	57.442	3.837	0.714	1.000
CB 3.128.2	29.830	30.185	4.018	0.600	0.833
CG 3.128.3	36.010	36.085	1.533	0.600	0.833
N 3.128.4	119.775	120.574	4.837	0.818	1.000
HA 3.128.5	3.908	4.245	0.429	0.500	1.000
HB2 3.128.6	1.901	2.021	0.233	0.600	0.833
HB3 3.128.7	1.954	1.994	0.244	0.400	0.833
HG 3.128.8	2.014	2.258	0.226	0.600	0.833
H 3.128.9	8.084	8.332	0.601	0.752	1.000
HE2	NA	—	—	0.000	0.000

3.128.1 Detailed Probabilities of GLU128CA:

Overall probability: 0.714
Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU127	1.00	1.00
GLU128	0.60	1.00

Expected NOESY Contacts

Proton	Expected probability
L127HA	1.00
E128HB2	1.00
E128HB3	1.00
E128HG2	1.00
E128H	1.00
E128HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU127	HA	1.00	0.007	1.00	0.07
LEU127	HB3	0.90	0.024	1.00	0.71
GLU128	HA	1.00	0.381	0.00	0.00
GLU128	HB2	1.00	0.005	1.00	0.87
GLU128	HB3	1.00	0.058	0.00	0.00
GLU128	HG2	1.00	0.020	1.00	0.65
GLU128	H	1.00	0.019	1.00	0.28

3.128.2 Detailed Probabilities of GLU128CB:

Overall probability: 0.600

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU128	0.60	0.83

Expected NOESY Contacts

Proton	Expected probability
E128HA	1.00
E128HB3	1.00
E128HG2	1.00
E128H	1.00
E128HE2	1.00
E128HB2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU128	HA	1.00	0.004	1.00	0.59
GLU128	HB2	1.00	0.003	1.00	14.73
GLU128	HB3	1.00	0.050	0.00	0.00
GLU128	HG2	1.00	0.110	0.00	0.00
GLU128	H	1.00	0.003	1.00	0.60

3.128.3 Detailed Probabilities of GLU128CG:

Overall probability: 0.600

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU128	0.60	0.83

Expected NOESY Contacts

Proton	Expected probability
E128HA	1.00
E128HB2	1.00
E128HB3	1.00
E128HG3	1.00
E128H	1.00
E128HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU128	HA	1.00	0.002	1.00	0.58
GLU128	HB2	1.00	0.123	0.00	0.00
GLU128	HB3	1.00	0.070	0.00	0.00
GLU128	HG2	1.00	0.010	1.00	20.76
GLU128	H	1.00	0.000	1.00	0.33

3.128.4 Detailed Probabilities of GLU128N:

Overall probability: 0.818

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU127	0.67	1.00
GLU128	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L127HA	1.00
L127HB2	1.00
L127HB3	1.00
L127HG	0.98
L127H	1.00
E128HA	1.00
E128HB2	1.00
E128HB3	1.00
E128HG2	1.00
E128H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU127	HA	1.00	0.059	0.00	0.00
LEU127	HB2	1.00	0.017	1.00	-1585593.00
LEU127	HB3	1.00	0.018	1.00	-892233.00
LEU127	HG	0.98	0.002	1.00	-207979.00
LEU127	H	1.00	0.064	0.00	0.00
LEU127	HD11	0.51	0.029	1.00	-143441.00
GLU128	HA	1.00	0.003	1.00	-608202.00
GLU128	HB2	1.00	0.015	1.00	-1585593.00
GLU128	HB3	1.00	0.028	1.00	-289522.00
GLU128	HG2	1.00	0.019	1.00	-904565.00
GLU128	H	1.00	0.028	1.00	-7986668.00

3.128.5 Detailed Probabilities of GLU128HA:

Overall probability: 0.500

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU127	0.00	1.00
GLU128	0.60	1.00

Expected NOESY Contacts

Proton	Expected probability
L127HA	1.00
E128HB2	1.00
E128HB3	1.00
E128HG2	1.00
E128H	1.00
E128HA	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU127	HA	1.00	0.814	0.00	0.00
GLU128	HA	1.00	0.381	0.00	0.00
GLU128	HB2	1.00	0.004	1.00	0.59
GLU128	HB3	1.00	0.050	0.00	0.00
GLU128	HG2	1.00	0.002	1.00	0.58
GLU128	H	1.00	0.003	1.00	-608202.00

3.128.6 Detailed Probabilities of GLU128HB2:

Overall probability: 0.600

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU128	0.60	0.83

Expected NOESY Contacts

Proton	Expected probability
E128HA	1.00
E128HB3	1.00
E128HG2	1.00
E128H	1.00
E128HE2	1.00
E128HB2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU128	HA	1.00	0.005	1.00	0.87
GLU128	HB2	1.00	0.003	1.00	14.73
GLU128	HB3	1.00	0.498	0.00	0.00
GLU128	HG2	1.00	0.123	0.00	0.00
GLU128	H	1.00	0.015	1.00	-1585593.00

3.128.7 Detailed Probabilities of GLU128HB3:

Overall probability: 0.400

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU128	0.40	0.83

Expected NOESY Contacts

Proton	Expected probability
E128HA	1.00
E128HB2	1.00
E128HG2	1.00
E128H	1.00
E128HE2	1.00
E128HB3	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU128	HA	1.00	0.058	0.00	0.00
GLU128	HB2	1.00	0.050	0.00	0.00
GLU128	HB3	1.00	0.004	1.00	11.43
GLU128	HG2	1.00	0.070	0.00	0.00
GLU128	H	1.00	0.028	1.00	-289522.00

3.128.8 Detailed Probabilities of GLU128HG2:

Overall probability: 0.600

Overall confidence: 0.833

Inter- and intra-residue probability

Residue	Probability	Confidence
GLU128	0.60	0.83

Expected NOESY Contacts

Proton	Expected probability
E128HA	1.00
E128HB2	1.00
E128HB3	1.00
E128HG3	1.00
E128H	1.00
E128HE2	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
GLU128	HA	1.00	0.020	1.00	0.65
GLU128	HB2	1.00	0.110	0.00	0.00
GLU128	HB3	1.00	0.611	0.00	0.00
GLU128	HG2	1.00	0.010	1.00	20.76
GLU128	H	1.00	0.019	1.00	-904565.00

3.128.9 Detailed Probabilities of GLU128H:

Overall probability: 0.752

Overall confidence: 1.000

Inter- and intra-residue probability

Residue	Probability	Confidence
LEU127	0.57	1.00
GLU128	1.00	1.00

Expected NOESY Contacts

Proton	Expected probability
L127HA	1.00
L127HB2	1.00
L127HB3	1.00
L127HG	0.98
L127H	1.00
E128HA	1.00
E128HB2	1.00
E128HB3	1.00
E128HG2	1.00
E128H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
LEU127	HA	1.00	0.003	1.00	0.42
LEU127	HB2	1.00	0.080	0.00	0.00
LEU127	HB3	1.00	0.164	0.00	0.00
LEU127	HG	0.98	0.080	0.02	0.00
LEU127	H	1.00	0.002	1.00	-703601.00
LEU127	HD11	0.51	0.004	1.00	0.07
LEU127	HD21	0.58	0.024	1.00	0.12
GLU128	HA	1.00	0.019	1.00	0.28
GLU128	HB2	1.00	0.003	1.00	0.60
GLU128	HB3	1.00	0.005	1.00	0.64
GLU128	HG2	1.00	0.000	1.00	0.33
GLU128	H	1.00	0.028	1.00	-7986668.00

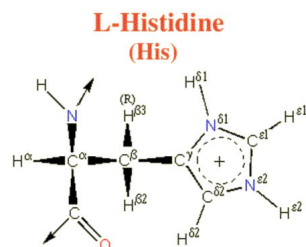
3.129 NA(129)**3.130 NA(130)****3.131 HIS(131)**

Figure 128: Image from the BMRB

Residue probability: 1.000

Residue probability confidence: 0.250

Chemical Shift Distributions and Assignment Probabilities

Atom	Assigned CS	DB avg.	DB std	Overall probability	Overall confidence
C	NA	—	—	0.000	0.000
CA	NA	—	—	0.000	0.000
CB	NA	—	—	0.000	0.000
CD2	NA	—	—	0.000	0.000
CE1	NA	—	—	0.000	0.000
N 3.131.1	125.272	119.696	4.105	1.000	0.250
ND1	NA	—	—	0.000	0.000
NE2	NA	—	—	0.000	0.000
HA	NA	—	—	0.000	0.000
HB	NA	—	—	0.000	0.000
HD2	NA	—	—	0.000	0.000
HE1	NA	—	—	0.000	0.000
H 3.131.2	8.059	8.260	0.687	1.000	0.250
HD1	NA	—	—	0.000	0.000
HE2	NA	—	—	0.000	0.000

3.131.1 Detailed Probabilities of HIS131N:

Overall probability: 1.000

Overall confidence: 0.250

Inter- and intra-residue probability

Residue	Probability	Confidence
HIS131	1.00	0.25

Expected NOESY Contacts

Proton	Expected probability
H131HA	1.00
H131HB2	1.00
H131HD1	0.96
H131H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
HIS131	H	1.00	0.002	1.00	-2351783.00

3.131.2 Detailed Probabilities of HIS131H:

Overall probability: 1.000

Overall confidence: 0.250

Inter- and intra-residue probability

Residue	Probability	Confidence
HIS131	1.00	0.25

Expected NOESY Contacts

Proton	Expected probability
H131HA	1.00
H131HB2	1.00
H131HD1	0.96
H131H	1.00

NOESY contacts detailed probability

Residue	Proton	Expected probability	Min PPM differences	Probability	Peak intensity ratio
HIS131	H	1.00	0.002	1.00	-2351783.00