Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	5LCS
Title	:	NMR structure of Chicken AvBD7 defensin
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Deposited on	:	2016-06-22

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

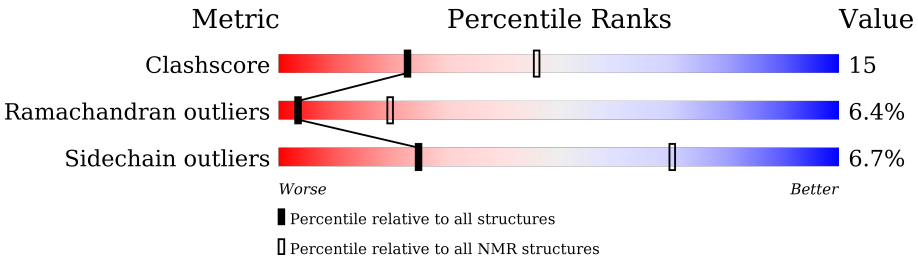
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027939
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	47	45% 40% 15%

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:8-A:47 (40)	0.34	8

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 733 atoms, of which 359 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Gallinacin-7.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	47	733	235	359	73	60	6	0

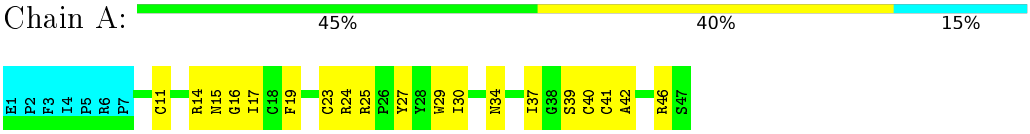
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Gallinacin-7

Chain A:



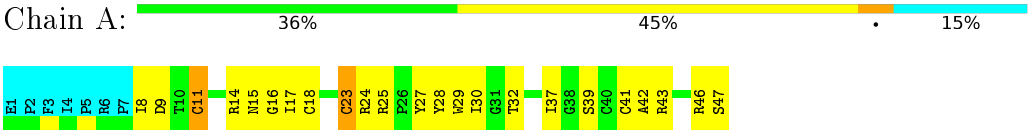
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Gallinacin-7

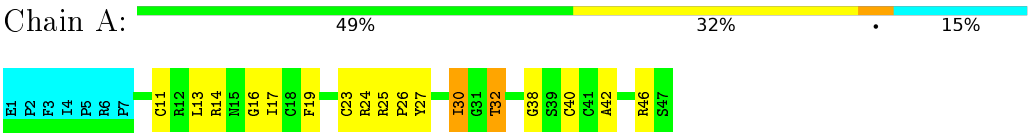
Chain A:



4.2.2 Score per residue for model 2

- Molecule 1: Gallinacin-7

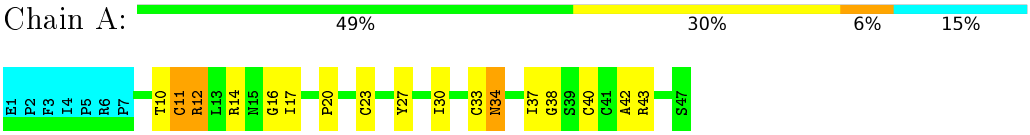
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Gallinacin-7

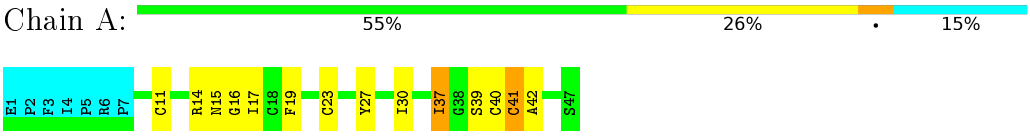
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Gallinacin-7

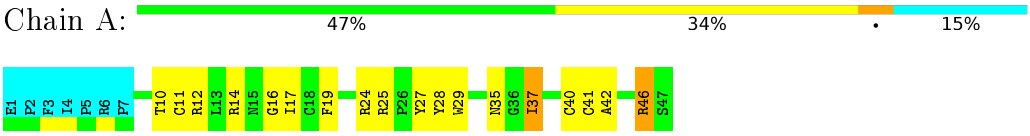
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Gallinacin-7

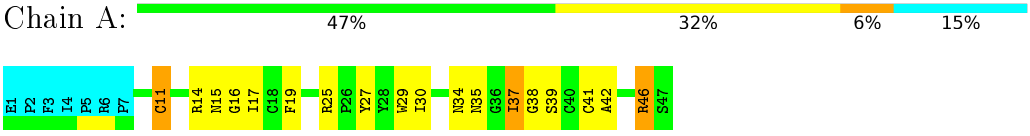
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Gallinacin-7

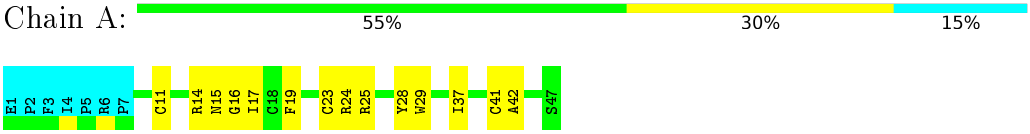
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Gallinacin-7

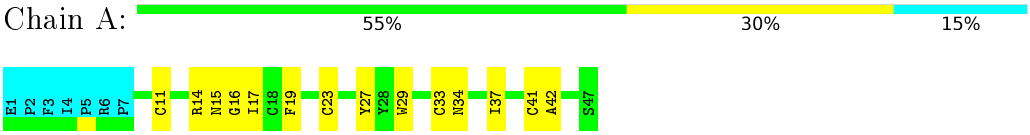
Chain A:



4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Gallinacin-7

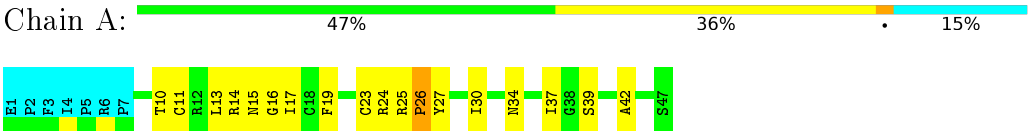
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: Gallinacin-7

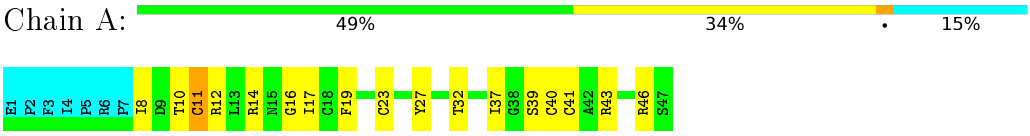
Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: Gallinacin-7

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 1000 calculated structures, 10 were deposited, based on the following criterion: *lowest energy and least restraints violations*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	5lcs_cs.cif
Number of chemical shift lists	1
Total number of shifts	502
Number of shifts mapped to atoms	0
Number of unparsed shifts	502
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.46±0.06	0±1/323 (0.1±0.2%)	0.54±0.02	0±0/434 (0.0±0.0%)
All	All	0.47	2/3230 (0.1%)	0.54	0/4340 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
All	All	0	1

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	28	TYR	CE2-CZ	5.59	1.45	1.38	7	1
1	A	28	TYR	CE1-CZ	-5.50	1.31	1.38	7	1

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	27	TYR	Sidechain	1

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	315	298	298	9±2
All	All	3150	2980	2980	90

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:SER:HB2	1:A:41:CYS:SG	0.67	2.28	10	2
1:A:14:ARG:HG3	1:A:15:ASN:N	0.65	2.06	8	6
1:A:16:GLY:O	1:A:17:ILE:HG12	0.64	1.92	3	4
1:A:24:ARG:O	1:A:25:ARG:HG2	0.64	1.92	1	4
1:A:14:ARG:HD3	1:A:40:CYS:SG	0.62	2.34	5	1
1:A:16:GLY:O	1:A:17:ILE:HG13	0.62	1.95	9	6
1:A:29:TRP:HA	1:A:41:CYS:SG	0.61	2.36	6	4
1:A:13:LEU:O	1:A:30:ILE:HD12	0.61	1.96	9	1
1:A:17:ILE:HD12	1:A:27:TYR:CE1	0.61	2.30	10	4
1:A:16:GLY:HA3	1:A:42:ALA:HA	0.58	1.74	7	9
1:A:14:ARG:HD2	1:A:40:CYS:SG	0.58	2.38	10	1
1:A:17:ILE:HG13	1:A:27:TYR:CE1	0.55	2.37	3	3
1:A:19:PHE:HB2	1:A:39:SER:OG	0.54	2.01	10	4
1:A:11:CYS:SG	1:A:14:ARG:HD3	0.52	2.44	3	1
1:A:10:THR:C	1:A:12:ARG:N	0.51	2.63	10	1
1:A:13:LEU:HD21	1:A:46:ARG:NH2	0.50	2.22	2	1
1:A:30:ILE:O	1:A:40:CYS:HB3	0.49	2.07	3	3
1:A:11:CYS:HB2	1:A:30:ILE:O	0.49	2.07	1	2
1:A:14:ARG:HA	1:A:14:ARG:NE	0.49	2.23	10	1
1:A:11:CYS:O	1:A:14:ARG:HG2	0.49	2.07	10	1
1:A:26:PRO:HD2	1:A:27:TYR:CE2	0.48	2.44	9	1
1:A:33:CYS:O	1:A:38:GLY:HA3	0.47	2.10	3	1
1:A:17:ILE:HG21	1:A:19:PHE:CE1	0.47	2.45	5	1
1:A:8:ILE:HA	1:A:46:ARG:HD2	0.46	1.87	10	1
1:A:27:TYR:CD1	1:A:43:ARG:HA	0.46	2.44	1	3
1:A:30:ILE:HG12	1:A:40:CYS:O	0.46	2.10	2	1
1:A:20:PRO:HB3	1:A:34:ASN:HD21	0.46	1.71	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:CYS:SG	1:A:29:TRP:HB2	0.45	2.52	1	1
1:A:14:ARG:CG	1:A:15:ASN:N	0.45	2.79	8	3
1:A:19:PHE:CD1	1:A:23:CYS:SG	0.45	3.09	9	3
1:A:19:PHE:HD1	1:A:23:CYS:SG	0.45	2.34	8	1
1:A:10:THR:C	1:A:12:ARG:H	0.44	2.15	10	3
1:A:19:PHE:HD1	1:A:41:CYS:SG	0.44	2.34	4	1
1:A:9:ASP:O	1:A:30:ILE:HG22	0.43	2.12	1	1
1:A:17:ILE:HG21	1:A:19:PHE:CZ	0.43	2.49	2	1
1:A:32:THR:HG22	1:A:38:GLY:O	0.42	2.13	2	1
1:A:14:ARG:HG3	1:A:15:ASN:H	0.42	1.74	6	1
1:A:28:TYR:CD1	1:A:46:ARG:HB3	0.41	2.50	1	1
1:A:28:TYR:CE1	1:A:46:ARG:HD2	0.41	2.50	5	1
1:A:43:ARG:HD3	1:A:43:ARG:C	0.41	2.36	3	1
1:A:33:CYS:SG	1:A:34:ASN:N	0.41	2.93	8	1
1:A:24:ARG:O	1:A:25:ARG:HG3	0.41	2.16	5	1
1:A:8:ILE:HG12	1:A:46:ARG:HG3	0.40	1.93	1	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	39/47 (83%)	27±2 (70±6%)	9±2 (24±6%)	3±1 (6±3%)	3	20
All	All	390/470 (83%)	273 (70%)	92 (24%)	25 (6%)	3	20

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	11	CYS	10
1	A	37	ILE	6
1	A	34	ASN	3
1	A	26	PRO	2
1	A	35	ASN	2
1	A	10	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	38	GLY	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	33/39 (85%)	31±1 (93±4%)	2±1 (7±4%)	25	70
All	All	330/390 (85%)	308 (93%)	22 (7%)	25	70

All 10 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	37	ILE	6
1	A	23	CYS	5
1	A	32	THR	3
1	A	46	ARG	2
1	A	30	ILE	1
1	A	14	ARG	1
1	A	18	CYS	1
1	A	25	ARG	1
1	A	12	ARG	1
1	A	41	CYS	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is

considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	PCA	A	1	1	7,8,9	0.79±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	PCA	A	1	1	9,10,12	1.72±0.04	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	A	1	1	-	0±0,0,11,13	0±0,1,1,1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no carbohydrates in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: 5lcs_cs.cif

Chemical shift list name: *shifts2.star*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	502
Number of shifts mapped to atoms	0
Number of unparsed shifts	502
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

- Entity instance (chain) must be specified. All 502 occurences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	1	PCA	CB	24.155	?	?
2	?	1	PCA	CG	29.208	?	?
3	?	1	PCA	HA	4.663	?	?
4	?	1	PCA	HB2	2.585	?	?
5	?	1	PCA	HB3	2.001	?	?
6	?	1	PCA	HG2	2.415	?	?
7	?	1	PCA	HG3	2.416	?	?
8	?	2	PRO	CA	60.483	?	?
9	?	2	PRO	CB	29.164	?	?
10	?	2	PRO	CD	47.362	?	?
11	?	2	PRO	CG	24.557	?	?
12	?	2	PRO	HA	4.415	?	?
13	?	2	PRO	HB2	2.232	?	?
14	?	2	PRO	HB3	1.817	?	?
15	?	2	PRO	HD2	3.692	?	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
16	?	2	PRO	HD3	3.600	?	?
17	?	2	PRO	HG2	1.991	?	?
18	?	2	PRO	HG3	1.991	?	?
19	?	3	PHE	CB	36.775	?	?
20	?	3	PHE	CZ	128.688	?	?
21	?	3	PHE	H	8.176	?	?
22	?	3	PHE	HA	4.595	?	?
23	?	3	PHE	HB2	3.111	?	?
24	?	3	PHE	HB3	2.996	?	?
25	?	3	PHE	HZ	7.336	?	?
26	?	3	PHE	N	120.027	?	?
27	?	3	PHE	HD1	7.214	?	?
28	?	3	PHE	HD2	7.214	?	?
29	?	3	PHE	HE1	7.315	?	?
30	?	3	PHE	HE2	7.315	?	?
31	?	3	PHE	CD1	129.135	?	?
32	?	3	PHE	CD2	129.135	?	?
33	?	4	ILE	CA	55.112	?	?
34	?	4	ILE	CB	36.274	?	?
35	?	4	ILE	CD1	10.268	?	?
36	?	4	ILE	CG1	24.264	?	?
37	?	4	ILE	CG2	14.104	?	?
38	?	4	ILE	H	7.916	?	?
39	?	4	ILE	HA	4.372	?	?
40	?	4	ILE	HB	1.727	?	?
41	?	4	ILE	HG12	1.410	?	?
42	?	4	ILE	HG13	1.073	?	?
43	?	4	ILE	N	126.519	?	?
44	?	4	ILE	HD11	0.839	?	?
45	?	4	ILE	HD12	0.839	?	?
46	?	4	ILE	HD13	0.839	?	?
47	?	4	ILE	HG21	0.838	?	?
48	?	4	ILE	HG22	0.838	?	?
49	?	4	ILE	HG23	0.838	?	?
50	?	5	PRO	CA	60.162	?	?
51	?	5	PRO	CB	29.348	?	?
52	?	5	PRO	CD	48.217	?	?
53	?	5	PRO	CG	24.540	?	?
54	?	5	PRO	HA	4.276	?	?
55	?	5	PRO	HB2	2.288	?	?
56	?	5	PRO	HB3	1.872	?	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
57	?	5	PRO	HD2	3.661	?	?
58	?	5	PRO	HD3	3.635	?	?
59	?	5	PRO	HG2	1.982	?	?
60	?	5	PRO	HG3	1.982	?	?
61	?	6	ARG	CB	27.236	?	?
62	?	6	ARG	CD	40.525	?	?
63	?	6	ARG	CG	24.259	?	?
64	?	6	ARG	H	8.317	?	?
65	?	6	ARG	HA	4.592	?	?
66	?	6	ARG	HD2	3.221	?	?
67	?	6	ARG	HD3	3.221	?	?
68	?	6	ARG	HE	7.195	?	?
69	?	6	ARG	HG2	1.716	?	?
70	?	6	ARG	HG3	1.716	?	?
71	?	6	ARG	N	122.140	?	?
72	?	6	ARG	HB2	1.831	?	?
73	?	6	ARG	HB3	1.831	?	?
74	?	7	PRO	CA	60.483	?	?
75	?	7	PRO	CB	29.334	?	?
76	?	7	PRO	CD	47.844	?	?
77	?	7	PRO	CG	24.534	?	?
78	?	7	PRO	HA	4.431	?	?
79	?	7	PRO	HB2	2.273	?	?
80	?	7	PRO	HB3	1.863	?	?
81	?	7	PRO	HD2	3.798	?	?
82	?	7	PRO	HD3	3.614	?	?
83	?	7	PRO	HG2	2.014	?	?
84	?	7	PRO	HG3	2.014	?	?
85	?	8	ILE	CA	58.282	?	?
86	?	8	ILE	CB	36.277	?	?
87	?	8	ILE	CD1	10.247	?	?
88	?	8	ILE	CG1	24.671	?	?
89	?	8	ILE	CG2	14.791	?	?
90	?	8	ILE	H	8.241	?	?
91	?	8	ILE	HA	4.086	?	?
92	?	8	ILE	HB	1.801	?	?
93	?	8	ILE	HG12	1.504	?	?
94	?	8	ILE	HG13	1.198	?	?
95	?	8	ILE	N	121.121	?	?
96	?	8	ILE	HD11	0.879	?	?
97	?	8	ILE	HD12	0.879	?	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
98	?	8	ILE	HD13	0.879	?	?
99	?	8	ILE	HG21	0.872	?	?
100	?	8	ILE	HG22	0.872	?	?
101	?	8	ILE	HG23	0.872	?	?
102	?	9	ASP	CA	50.651	?	?
103	?	9	ASP	CB	38.673	?	?
104	?	9	ASP	H	8.322	?	?
105	?	9	ASP	HA	4.764	?	?
106	?	9	ASP	HB2	2.865	?	?
107	?	9	ASP	HB3	2.666	?	?
108	?	9	ASP	N	125.097	?	?
109	?	10	THR	CA	61.403	?	?
110	?	10	THR	CB	65.998	?	?
111	?	10	THR	CG2	19.280	?	?
112	?	10	THR	H	8.359	?	?
113	?	10	THR	HA	3.981	?	?
114	?	10	THR	HB	4.312	?	?
115	?	10	THR	N	116.733	?	?
116	?	10	THR	HG21	1.242	?	?
117	?	10	THR	HG22	1.242	?	?
118	?	10	THR	HG23	1.242	?	?
119	?	11	CYS	H	8.444	?	?
120	?	11	CYS	HA	4.368	?	?
121	?	11	CYS	HB2	3.081	?	?
122	?	11	CYS	HB3	3.079	?	?
123	?	11	CYS	N	121.430	?	?
124	?	12	ARG	CA	56.070	?	?
125	?	12	ARG	CB	27.236	?	?
126	?	12	ARG	CD	40.469	?	?
127	?	12	ARG	CG	24.238	?	?
128	?	12	ARG	H	8.026	?	?
129	?	12	ARG	HA	4.206	?	?
130	?	12	ARG	HB2	1.834	?	?
131	?	12	ARG	HB3	1.834	?	?
132	?	12	ARG	HD2	3.273	?	?
133	?	12	ARG	HD3	3.235	?	?
134	?	12	ARG	HE	7.292	?	?
135	?	12	ARG	HG2	1.725	?	?
136	?	12	ARG	HG3	1.671	?	?
137	?	12	ARG	N	120.427	?	?
138	?	13	LEU	CA	54.628	?	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
139	?	13	LEU	CB	39.304	?	?
140	?	13	LEU	H	7.884	?	?
141	?	13	LEU	HA	4.129	?	?
142	?	13	LEU	HB2	1.750	?	?
143	?	13	LEU	HB3	1.652	?	?
144	?	13	LEU	HG	1.654	?	?
145	?	13	LEU	N	120.239	?	?
146	?	13	LEU	HD11	0.882	?	?
147	?	13	LEU	HD12	0.882	?	?
148	?	13	LEU	HD13	0.882	?	?
149	?	13	LEU	HD21	0.882	?	?
150	?	13	LEU	HD22	0.882	?	?
151	?	13	LEU	HD23	0.882	?	?
152	?	14	ARG	CA	52.679	?	?
153	?	14	ARG	CD	41.049	?	?
154	?	14	ARG	H	7.239	?	?
155	?	14	ARG	HA	4.337	?	?
156	?	14	ARG	HB2	2.044	?	?
157	?	14	ARG	HB3	1.595	?	?
158	?	14	ARG	HD2	3.099	?	?
159	?	14	ARG	HD3	3.099	?	?
160	?	14	ARG	HE	6.993	?	?
161	?	14	ARG	HG2	1.741	?	?
162	?	14	ARG	HG3	1.741	?	?
163	?	14	ARG	N	117.284	?	?
164	?	15	ASN	CA	51.678	?	?
165	?	15	ASN	CB	34.191	?	?
166	?	15	ASN	H	8.007	?	?
167	?	15	ASN	HA	4.410	?	?
168	?	15	ASN	HB2	3.147	?	?
169	?	15	ASN	HB3	2.912	?	?
170	?	15	ASN	HD21	7.530	?	?
171	?	15	ASN	HD22	6.882	?	?
172	?	15	ASN	N	112.907	?	?
173	?	16	GLY	H	8.005	?	?
174	?	16	GLY	HA2	4.511	?	?
175	?	16	GLY	HA3	3.239	?	?
176	?	16	GLY	N	105.090	?	?
177	?	17	ILE	CA	56.875	?	?
178	?	17	ILE	CB	38.674	?	?
179	?	17	ILE	CD1	10.183	?	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
180	?	17	ILE	CG1	24.598	?	?
181	?	17	ILE	CG2	15.058	?	?
182	?	17	ILE	H	8.677	?	?
183	?	17	ILE	HA	4.088	?	?
184	?	17	ILE	HB	1.484	?	?
185	?	17	ILE	N	119.314	?	?
186	?	17	ILE	HD11	0.811	?	?
187	?	17	ILE	HD12	0.811	?	?
188	?	17	ILE	HD13	0.811	?	?
189	?	17	ILE	HG12	1.045	?	?
190	?	17	ILE	HG13	1.045	?	?
191	?	17	ILE	HG21	0.326	?	?
192	?	17	ILE	HG22	0.326	?	?
193	?	17	ILE	HG23	0.326	?	?
194	?	18	CYS	CA	51.783	?	?
195	?	18	CYS	CB	37.977	?	?
196	?	18	CYS	H	8.571	?	?
197	?	18	CYS	HA	5.220	?	?
198	?	18	CYS	HB2	2.831	?	?
199	?	18	CYS	HB3	2.831	?	?
200	?	18	CYS	N	125.455	?	?
201	?	19	PHE	CA	52.612	?	?
202	?	19	PHE	CB	40.386	?	?
203	?	19	PHE	CZ	126.756	?	?
204	?	19	PHE	H	9.815	?	?
205	?	19	PHE	HA	4.821	?	?
206	?	19	PHE	HB2	3.071	?	?
207	?	19	PHE	HB3	2.817	?	?
208	?	19	PHE	HZ	6.480	?	?
209	?	19	PHE	N	131.725	?	?
210	?	19	PHE	HD1	7.151	?	?
211	?	19	PHE	HD2	7.151	?	?
212	?	19	PHE	HE1	6.808	?	?
213	?	19	PHE	HE2	6.808	?	?
214	?	19	PHE	CD1	129.433	?	?
215	?	19	PHE	CD2	129.433	?	?
216	?	19	PHE	CE1	128.080	?	?
217	?	19	PHE	CE2	128.080	?	?
218	?	20	PRO	CA	60.406	?	?
219	?	20	PRO	CB	28.232	?	?
220	?	20	PRO	CD	47.673	?	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
221	?	20	PRO	CG	24.434	?	?
222	?	20	PRO	HA	4.677	?	?
223	?	20	PRO	HD2	3.775	?	?
224	?	20	PRO	HD3	3.709	?	?
225	?	20	PRO	HG2	2.064	?	?
226	?	20	PRO	HG3	2.064	?	?
227	?	20	PRO	HB2	2.169	?	?
228	?	20	PRO	HB3	2.169	?	?
229	?	21	GLY	CA	42.288	?	?
230	?	21	GLY	H	8.001	?	?
231	?	21	GLY	HA2	4.206	?	?
232	?	21	GLY	HA3	3.892	?	?
233	?	21	GLY	N	109.553	?	?
234	?	22	ILE	CA	57.663	?	?
235	?	22	ILE	CB	37.337	?	?
236	?	22	ILE	CD1	10.268	?	?
237	?	22	ILE	CG1	23.721	?	?
238	?	22	ILE	CG2	14.870	?	?
239	?	22	ILE	H	7.835	?	?
240	?	22	ILE	HA	4.419	?	?
241	?	22	ILE	HB	1.929	?	?
242	?	22	ILE	HG12	1.300	?	?
243	?	22	ILE	HG13	1.161	?	?
244	?	22	ILE	N	118.232	?	?
245	?	22	ILE	HD11	0.840	?	?
246	?	22	ILE	HD12	0.840	?	?
247	?	22	ILE	HD13	0.840	?	?
248	?	22	ILE	HG21	0.939	?	?
249	?	22	ILE	HG22	0.939	?	?
250	?	22	ILE	HG23	0.939	?	?
251	?	23	CYS	CA	50.918	?	?
252	?	23	CYS	CB	36.430	?	?
253	?	23	CYS	H	8.653	?	?
254	?	23	CYS	HA	4.230	?	?
255	?	23	CYS	HB2	2.750	?	?
256	?	23	CYS	HB3	2.476	?	?
257	?	23	CYS	N	119.505	?	?
258	?	24	ARG	CA	51.319	?	?
259	?	24	ARG	CB	29.307	?	?
260	?	24	ARG	CD	40.541	?	?
261	?	24	ARG	CG	24.411	?	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
262	?	24	ARG	H	7.981	?	?
263	?	24	ARG	HA	4.574	?	?
264	?	24	ARG	HE	7.210	?	?
265	?	24	ARG	HG2	1.612	?	?
266	?	24	ARG	HG3	1.609	?	?
267	?	24	ARG	N	123.459	?	?
268	?	24	ARG	HB2	1.815	?	?
269	?	24	ARG	HB3	1.815	?	?
270	?	24	ARG	HD2	3.184	?	?
271	?	24	ARG	HD3	3.184	?	?
272	?	25	ARG	CA	53.161	?	?
273	?	25	ARG	CB	26.641	?	?
274	?	25	ARG	HA	4.294	?	?
275	?	25	ARG	HB2	1.742	?	?
276	?	25	ARG	HB3	1.742	?	?
277	?	25	ARG	HE	7.131	?	?
278	?	25	ARG	HG2	1.566	?	?
279	?	25	ARG	HG3	1.561	?	?
280	?	25	ARG	HD2	3.089	?	?
281	?	25	ARG	HD3	3.089	?	?
282	?	26	PRO	CA	61.318	?	?
283	?	26	PRO	CB	29.346	?	?
284	?	26	PRO	CD	47.561	?	?
285	?	26	PRO	CG	24.390	?	?
286	?	26	PRO	HA	4.447	?	?
287	?	26	PRO	HB2	2.282	?	?
288	?	26	PRO	HB3	1.861	?	?
289	?	26	PRO	HD2	3.514	?	?
290	?	26	PRO	HD3	3.514	?	?
291	?	26	PRO	HG2	2.105	?	?
292	?	26	PRO	HG3	1.072	?	?
293	?	27	TYR	CA	55.703	?	?
294	?	27	TYR	H	9.334	?	?
295	?	27	TYR	HA	5.048	?	?
296	?	27	TYR	HB2	3.036	?	?
297	?	27	TYR	HB3	2.680	?	?
298	?	27	TYR	N	127.346	?	?
299	?	27	TYR	HD1	6.936	?	?
300	?	27	TYR	HD2	6.936	?	?
301	?	27	TYR	HE1	6.872	?	?
302	?	27	TYR	HE2	6.872	?	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
303	?	27	TYR	CD1	130.296	?	?
304	?	27	TYR	CD2	130.296	?	?
305	?	27	TYR	CE1	115.857	?	?
306	?	27	TYR	CE2	115.857	?	?
307	?	28	TYR	CA	53.173	?	?
308	?	28	TYR	H	9.092	?	?
309	?	28	TYR	HA	4.891	?	?
310	?	28	TYR	HB2	3.076	?	?
311	?	28	TYR	HB3	2.968	?	?
312	?	28	TYR	N	116.456	?	?
313	?	28	TYR	HD1	6.994	?	?
314	?	28	TYR	HD2	6.994	?	?
315	?	28	TYR	HE1	6.585	?	?
316	?	28	TYR	HE2	6.585	?	?
317	?	28	TYR	CD1	131.434	?	?
318	?	28	TYR	CD2	131.434	?	?
319	?	28	TYR	CE1	115.047	?	?
320	?	28	TYR	CE2	115.047	?	?
321	?	29	TRP	CA	57.954	?	?
322	?	29	TRP	CB	28.171	?	?
323	?	29	TRP	CD1	125.639	?	?
324	?	29	TRP	CE3	118.393	?	?
325	?	29	TRP	CH2	121.867	?	?
326	?	29	TRP	CZ2	111.671	?	?
327	?	29	TRP	CZ3	119.239	?	?
328	?	29	TRP	H	8.867	?	?
329	?	29	TRP	HA	4.710	?	?
330	?	29	TRP	HB2	3.373	?	?
331	?	29	TRP	HB3	3.307	?	?
332	?	29	TRP	HD1	7.429	?	?
333	?	29	TRP	HE1	10.209	?	?
334	?	29	TRP	HE3	7.463	?	?
335	?	29	TRP	HH2	7.189	?	?
336	?	29	TRP	HZ2	7.357	?	?
337	?	29	TRP	HZ3	7.083	?	?
338	?	29	TRP	N	124.312	?	?
339	?	29	TRP	NE1	131.779	?	?
340	?	30	ILE	CA	58.257	?	?
341	?	30	ILE	CB	37.670	?	?
342	?	30	ILE	CD1	12.179	?	?
343	?	30	ILE	CG1	23.520	?	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
344	?	30	ILE	CG2	16.108	?	?
345	?	30	ILE	H	8.621	?	?
346	?	30	ILE	HA	4.561	?	?
347	?	30	ILE	HB	1.940	?	?
348	?	30	ILE	HG12	0.514	?	?
349	?	30	ILE	HG13	0.514	?	?
350	?	30	ILE	N	118.022	?	?
351	?	30	ILE	HD11	0.617	?	?
352	?	30	ILE	HD12	0.617	?	?
353	?	30	ILE	HD13	0.617	?	?
354	?	30	ILE	HG21	0.827	?	?
355	?	30	ILE	HG22	0.827	?	?
356	?	30	ILE	HG23	0.827	?	?
357	?	31	GLY	H	5.910	?	?
358	?	31	GLY	HA2	3.718	?	?
359	?	31	GLY	HA3	2.980	?	?
360	?	32	THR	CA	57.678	?	?
361	?	32	THR	CB	68.746	?	?
362	?	32	THR	CG2	18.914	?	?
363	?	32	THR	H	8.265	?	?
364	?	32	THR	HA	4.956	?	?
365	?	32	THR	HB	4.317	?	?
366	?	32	THR	N	110.239	?	?
367	?	32	THR	HG21	1.535	?	?
368	?	32	THR	HG22	1.535	?	?
369	?	32	THR	HG23	1.535	?	?
370	?	33	CYS	CA	54.044	?	?
371	?	33	CYS	H	7.829	?	?
372	?	33	CYS	HA	4.852	?	?
373	?	33	CYS	HB2	3.500	?	?
374	?	33	CYS	HB3	3.264	?	?
375	?	33	CYS	N	114.880	?	?
376	?	34	ASN	CA	51.260	?	?
377	?	34	ASN	CB	34.391	?	?
378	?	34	ASN	H	9.223	?	?
379	?	34	ASN	HA	4.390	?	?
380	?	34	ASN	HB2	3.040	?	?
381	?	34	ASN	HB3	2.582	?	?
382	?	34	ASN	HD21	7.504	?	?
383	?	34	ASN	HD22	6.879	?	?
384	?	34	ASN	N	119.258	?	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
385	?	34	ASN	ND2	112.686	?	?
386	?	35	ASN	CA	51.620	?	?
387	?	35	ASN	CB	34.709	?	?
388	?	35	ASN	H	8.950	?	?
389	?	35	ASN	HA	4.328	?	?
390	?	35	ASN	HB2	3.053	?	?
391	?	35	ASN	HB3	2.827	?	?
392	?	35	ASN	HD21	7.557	?	?
393	?	35	ASN	HD22	6.879	?	?
394	?	35	ASN	N	115.216	?	?
395	?	35	ASN	ND2	113.198	?	?
396	?	36	GLY	H	7.800	?	?
397	?	36	GLY	HA2	4.381	?	?
398	?	36	GLY	HA3	3.613	?	?
399	?	36	GLY	N	104.391	?	?
400	?	37	ILE	CA	59.028	?	?
401	?	37	ILE	CB	36.201	?	?
402	?	37	ILE	CD1	10.247	?	?
403	?	37	ILE	CG1	24.257	?	?
404	?	37	ILE	CG2	14.933	?	?
405	?	37	ILE	H	7.509	?	?
406	?	37	ILE	HA	4.391	?	?
407	?	37	ILE	HB	2.128	?	?
408	?	37	ILE	HG12	1.491	?	?
409	?	37	ILE	HG13	1.366	?	?
410	?	37	ILE	N	117.474	?	?
411	?	37	ILE	HD11	0.889	?	?
412	?	37	ILE	HD12	0.889	?	?
413	?	37	ILE	HD13	0.889	?	?
414	?	37	ILE	HG21	0.979	?	?
415	?	37	ILE	HG22	0.979	?	?
416	?	37	ILE	HG23	0.979	?	?
417	?	38	GLY	H	8.245	?	?
418	?	38	GLY	HA2	4.620	?	?
419	?	38	GLY	HA3	3.709	?	?
420	?	38	GLY	N	109.137	?	?
421	?	39	SER	CB	63.056	?	?
422	?	39	SER	H	8.966	?	?
423	?	39	SER	HA	4.837	?	?
424	?	39	SER	HB2	4.009	?	?
425	?	39	SER	HB3	3.937	?	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
426	?	39	SER	HG	5.761	?	?
427	?	39	SER	N	117.008	?	?
428	?	40	CYS	H	8.801	?	?
429	?	40	CYS	HA	4.804	?	?
430	?	40	CYS	HB2	2.214	?	?
431	?	40	CYS	HB3	2.093	?	?
432	?	40	CYS	N	125.428	?	?
433	?	41	CYS	CA	49.756	?	?
434	?	41	CYS	H	9.246	?	?
435	?	41	CYS	HA	5.535	?	?
436	?	41	CYS	HB2	2.990	?	?
437	?	41	CYS	HB3	2.686	?	?
438	?	41	CYS	N	127.164	?	?
439	?	42	ALA	CA	47.606	?	?
440	?	42	ALA	CB	19.585	?	?
441	?	42	ALA	H	9.042	?	?
442	?	42	ALA	HA	4.927	?	?
443	?	42	ALA	N	125.603	?	?
444	?	42	ALA	HB1	1.070	?	?
445	?	42	ALA	HB2	1.070	?	?
446	?	42	ALA	HB3	1.070	?	?
447	?	43	ARG	CD	40.230	?	?
448	?	43	ARG	CG	24.517	?	?
449	?	43	ARG	H	8.710	?	?
450	?	43	ARG	HA	4.155	?	?
451	?	43	ARG	HB2	1.517	?	?
452	?	43	ARG	HB3	1.442	?	?
453	?	43	ARG	HD2	2.820	?	?
454	?	43	ARG	HD3	2.757	?	?
455	?	43	ARG	HE	7.006	?	?
456	?	43	ARG	HG2	1.277	?	?
457	?	43	ARG	HG3	1.069	?	?
458	?	43	ARG	N	119.494	?	?
459	?	44	GLY	CA	42.225	?	?
460	?	44	GLY	H	8.465	?	?
461	?	44	GLY	HA2	4.224	?	?
462	?	44	GLY	HA3	3.888	?	?
463	?	44	GLY	N	112.215	?	?
464	?	45	TRP	CA	54.786	?	?
465	?	45	TRP	CB	27.140	?	?
466	?	45	TRP	CD1	124.518	?	?

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
467	?	45	TRP	CE3	118.143	?	?
468	?	45	TRP	CH2	121.867	?	?
469	?	45	TRP	CZ2	111.843	?	?
470	?	45	TRP	CZ3	119.239	?	?
471	?	45	TRP	H	8.145	?	?
472	?	45	TRP	HA	4.584	?	?
473	?	45	TRP	HB2	3.255	?	?
474	?	45	TRP	HB3	3.184	?	?
475	?	45	TRP	HD1	7.225	?	?
476	?	45	TRP	HE1	10.095	?	?
477	?	45	TRP	HE3	7.565	?	?
478	?	45	TRP	HH2	7.191	?	?
479	?	45	TRP	HZ2	7.466	?	?
480	?	45	TRP	HZ3	7.069	?	?
481	?	45	TRP	N	120.831	?	?
482	?	45	TRP	NE1	129.415	?	?
483	?	46	ARG	CB	28.275	?	?
484	?	46	ARG	CD	40.493	?	?
485	?	46	ARG	CG	24.034	?	?
486	?	46	ARG	H	7.973	?	?
487	?	46	ARG	HA	4.238	?	?
488	?	46	ARG	HB2	1.734	?	?
489	?	46	ARG	HB3	1.546	?	?
490	?	46	ARG	HD2	3.033	?	?
491	?	46	ARG	HD3	3.033	?	?
492	?	46	ARG	HE	7.064	?	?
493	?	46	ARG	HG2	1.366	?	?
494	?	46	ARG	HG3	1.366	?	?
495	?	46	ARG	N	122.395	?	?
496	?	47	SER	CA	57.254	?	?
497	?	47	SER	CB	61.971	?	?
498	?	47	SER	H	7.857	?	?
499	?	47	SER	HA	4.154	?	?
500	?	47	SER	HB2	3.814	?	?
501	?	47	SER	HB3	3.814	?	?
502	?	47	SER	N	122.525	?	?

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 499. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/196 (0%)	0/78 (0%)	0/80 (0%)	0/38 (0%)
Sidechain	0/254 (0%)	0/153 (0%)	0/80 (0%)	0/21 (0%)
Aromatic	0/49 (0%)	0/25 (0%)	0/22 (0%)	0/2 (0%)
Overall	0/499 (0%)	0/256 (0%)	0/182 (0%)	0/61 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 589. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/220 (0%)	0/87 (0%)	0/92 (0%)	0/41 (0%)
Sidechain	0/311 (0%)	0/189 (0%)	0/98 (0%)	0/24 (0%)
Aromatic	0/58 (0%)	0/30 (0%)	0/26 (0%)	0/2 (0%)
Overall	0/589 (0%)	0/306 (0%)	0/216 (0%)	0/67 (0%)

7.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots

No *random coil index* (RCI) plot could be generated from the current chemical shift list (shifts2.star). RCI is only applicable to proteins.