



# Full wwPDB NMR Structure Validation Report ⓘ

Nov 27, 2017 – 12:34 PM EST

PDB ID : 5L7M  
Title : Murin CXCL13 solution structure  
Authors : Monneau, Y.R.; Lortat-Jacob, H.  
Deposited on : unknown

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20030345  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

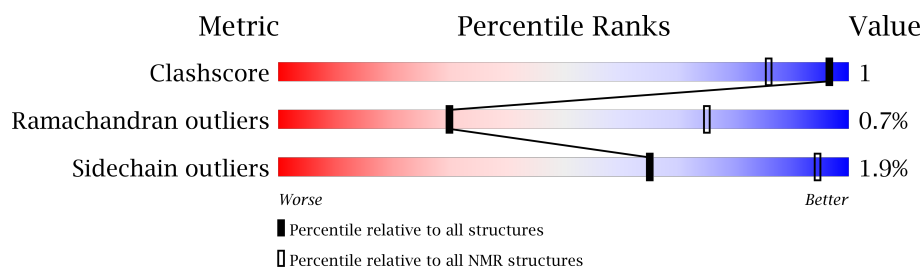
# 1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	88	 66% 34%

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 7 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:13-A:70 (58)	0.68	7

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 3 clusters and 4 single-model clusters were found.

Cluster number	Models
1	5, 7, 12, 13, 18, 19
2	4, 6, 8, 14, 15, 16
3	2, 9, 11, 20
Single-model clusters	1; 3; 10; 17

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1424 atoms, of which 739 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called C-X-C motif chemokine 13.

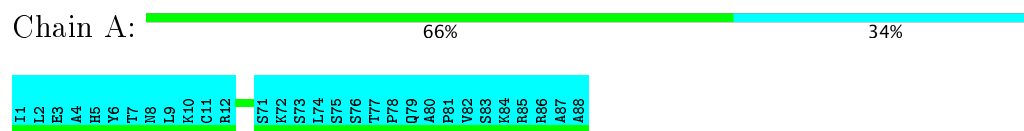
Mol	Chain	Residues	Atoms						Trace
1	A	88	Total	C	H	N	O	S	0
			1424	432	739	131	117	5	

## 4 Residue-property plots [i](#)

### 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: C-X-C motif chemokine 13

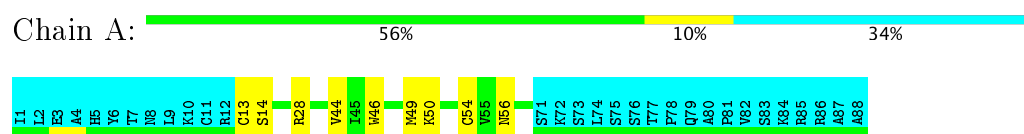


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

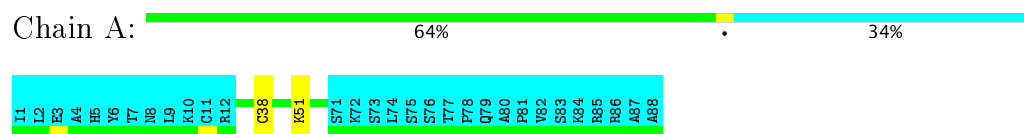
#### 4.2.1 Score per residue for model 1

- Molecule 1: C-X-C motif chemokine 13



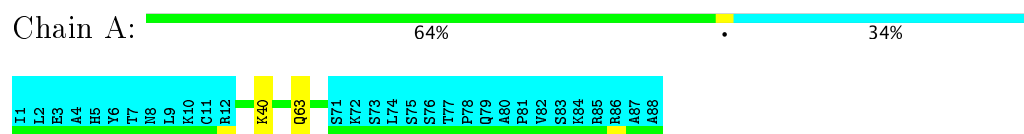
#### 4.2.2 Score per residue for model 2

- Molecule 1: C-X-C motif chemokine 13



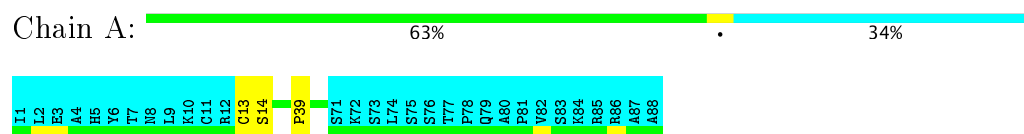
### 4.2.3 Score per residue for model 3

- Molecule 1: C-X-C motif chemokine 13



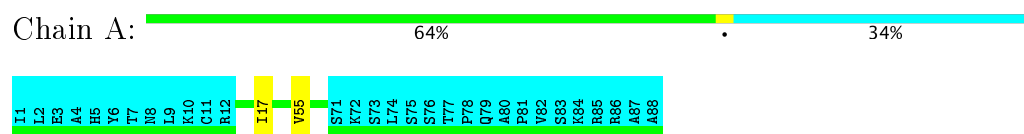
### 4.2.8 Score per residue for model 8

- Molecule 1: C-X-C motif chemokine 13



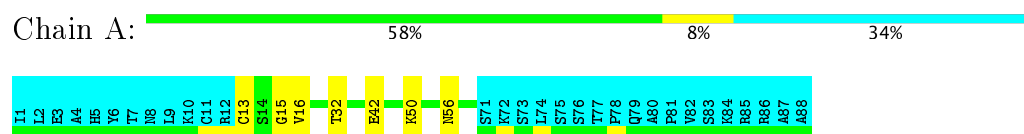
### 4.2.9 Score per residue for model 9

- Molecule 1: C-X-C motif chemokine 13



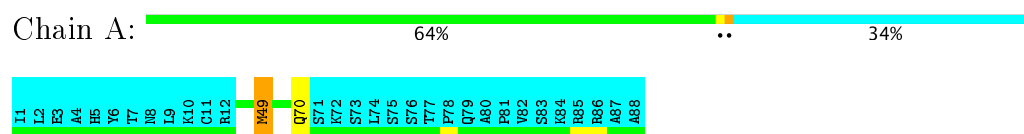
### 4.2.10 Score per residue for model 10

- Molecule 1: C-X-C motif chemokine 13



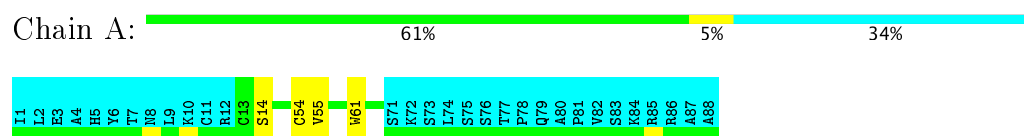
### 4.2.11 Score per residue for model 11

- Molecule 1: C-X-C motif chemokine 13



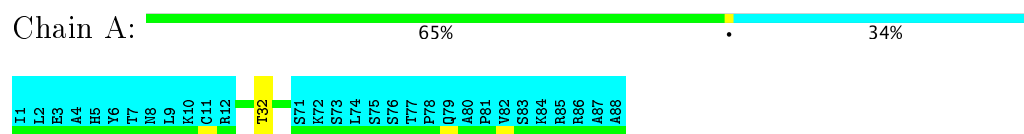
### 4.2.12 Score per residue for model 12

- Molecule 1: C-X-C motif chemokine 13



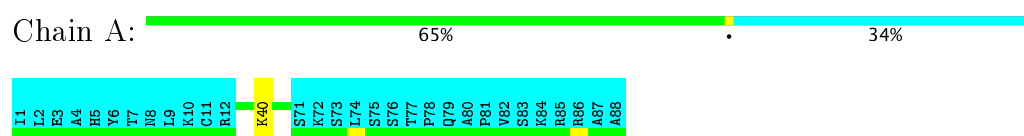
### 4.2.13 Score per residue for model 13

- Molecule 1: C-X-C motif chemokine 13



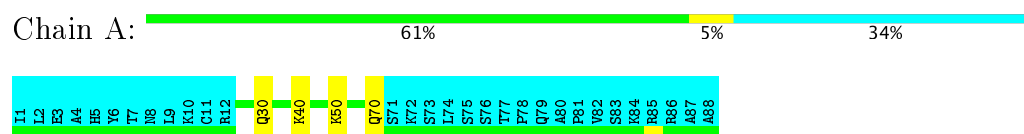
### 4.2.14 Score per residue for model 14

- Molecule 1: C-X-C motif chemokine 13



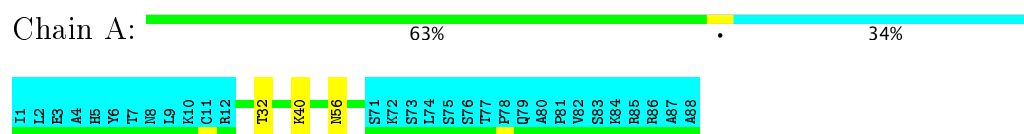
### 4.2.15 Score per residue for model 15

- Molecule 1: C-X-C motif chemokine 13



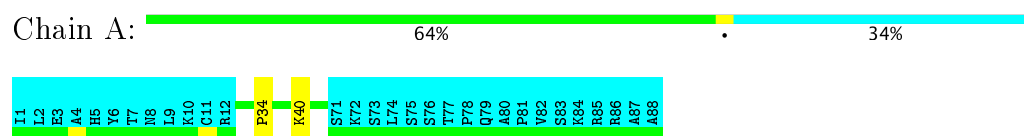
### 4.2.16 Score per residue for model 16

- Molecule 1: C-X-C motif chemokine 13



### 4.2.17 Score per residue for model 17

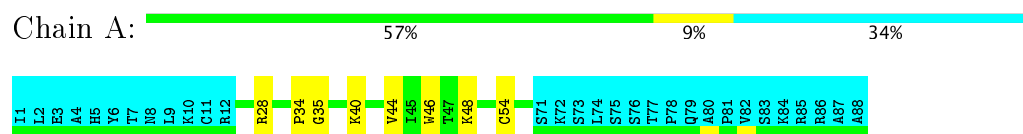
- Molecule 1: C-X-C motif chemokine 13





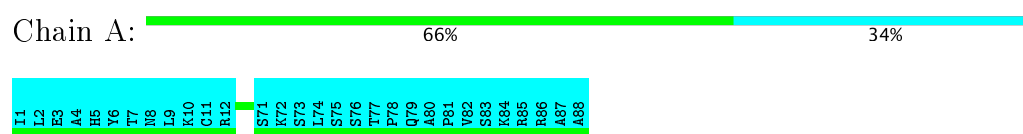
#### 4.2.18 Score per residue for model 18

- Molecule 1: C-X-C motif chemokine 13



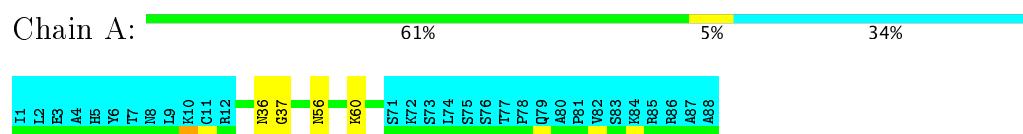
#### 4.2.19 Score per residue for model 19

- Molecule 1: C-X-C motif chemokine 13



#### 4.2.20 Score per residue for model 20

- Molecule 1: C-X-C motif chemokine 13



## 5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	
CYANA	structure calculation	

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)	5l7m_cs.cif
Number of chemical shift lists	1
Total number of shifts	996
Number of shifts mapped to atoms	0
Number of unparsed shifts	996
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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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	453	492	491	1±1
All	All	9060	9840	9820	17

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:CYS:SG	1:A:16:VAL:HG22	0.56	2.40	10	1
1:A:60:LYS:HA	1:A:63:GLN:HE21	0.50	1.67	7	1
1:A:49:MET:SD	1:A:49:MET:N	0.49	2.86	11	1
1:A:44:VAL:HG12	1:A:54:CYS:SG	0.47	2.50	18	1
1:A:49:MET:N	1:A:49:MET:SD	0.46	2.89	1	1
1:A:55:VAL:HG11	1:A:61:TRP:HE1	0.45	1.71	12	1
1:A:32:THR:HB	1:A:42:GLU:HB3	0.43	1.90	10	1
1:A:28:ARG:HG2	1:A:46:TRP:HB2	0.43	1.87	18	2
1:A:13:CYS:SG	1:A:14:SER:N	0.42	2.92	1	2
1:A:44:VAL:HG22	1:A:54:CYS:SG	0.42	2.54	1	1
1:A:14:SER:H	1:A:54:CYS:HB2	0.42	1.75	12	1
1:A:17:ILE:HD11	1:A:55:VAL:HG12	0.42	1.91	9	1
1:A:40:LYS:HA	1:A:40:LYS:HE2	0.41	1.92	16	1
1:A:63:GLN:O	1:A:67:ARG:HG2	0.41	2.15	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:VAL:HA	1:A:54:CYS:SG	0.40	2.56	5	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	58/88 (66%)	56±1 (96±2%)	2±1 (3±2%)	0±1 (1±1%)	30	75
All	All	1160/1760 (66%)	1114 (96%)	38 (3%)	8 (1%)	30	75

All 4 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	34	PRO	3
1	A	35	GLY	2
1	A	39	PRO	2
1	A	15	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	53/79 (67%)	52±1 (98±2%)	1±1 (2±2%)	65	94
All	All	1060/1580 (67%)	1040 (98%)	20 (2%)	65	94

All 11 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	56	ASN	4
1	A	40	LYS	4
1	A	50	LYS	3
1	A	70	GLN	2
1	A	30	GLN	1
1	A	67	ARG	1
1	A	49	MET	1
1	A	63	GLN	1
1	A	51	LYS	1
1	A	60	LYS	1
1	A	48	LYS	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 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 [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

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: 5l7m\_cs.cif

Chemical shift list name: *assigned\_chemical\_shifts*

#### 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	996
Number of shifts mapped to atoms	0
Number of unparsed shifts	996
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 996 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	2	LEU	C	176.822	?	1
2	?	2	LEU	HA	4.373	?	1
3	?	2	LEU	HB2	1.663	?	2
4	?	2	LEU	HB3	1.546	?	2
5	?	2	LEU	HG	1.588	?	1
6	?	2	LEU	HD11	0.827	?	2
7	?	2	LEU	HD12	0.827	?	2
8	?	2	LEU	HD13	0.827	?	2
9	?	2	LEU	HD21	0.892	?	2
10	?	2	LEU	HD22	0.892	?	2
11	?	2	LEU	HD23	0.892	?	2
12	?	2	LEU	CA	54.979	?	1
13	?	2	LEU	CB	42.444	?	1
14	?	2	LEU	CG	27.097	?	1
15	?	2	LEU	CD1	23.911	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
16	?	2	LEU	CD2	25.070	?	2
17	?	3	GLU	C	175.908	?	1
18	?	3	GLU	H	8.315	?	1
19	?	3	GLU	HA	4.208	?	1
20	?	3	GLU	HB2	1.973	?	2
21	?	3	GLU	HB3	1.884	?	2
22	?	3	GLU	HG2	2.214	?	1
23	?	3	GLU	HG3	2.214	?	1
24	?	3	GLU	CA	56.517	?	1
25	?	3	GLU	CB	30.398	?	1
26	?	3	GLU	CG	36.402	?	1
27	?	3	GLU	N	122.630	?	1
28	?	4	ALA	C	177.163	?	1
29	?	4	ALA	H	8.207	?	1
30	?	4	ALA	HA	4.197	?	1
31	?	4	ALA	HB1	1.240	?	1
32	?	4	ALA	HB2	1.240	?	1
33	?	4	ALA	HB3	1.240	?	1
34	?	4	ALA	CA	52.577	?	1
35	?	4	ALA	CB	19.237	?	1
36	?	4	ALA	N	125.023	?	1
37	?	5	HIS	C	174.538	?	1
38	?	5	HIS	H	8.228	?	1
39	?	5	HIS	HD2	7.048	?	1
40	?	5	HIS	HE1	8.303	?	1
41	?	5	HIS	CA	55.657	?	1
42	?	5	HIS	CB	29.862	?	1
43	?	5	HIS	CD2	119.567	?	1
44	?	5	HIS	CE1	136.822	?	1
45	?	5	HIS	N	117.868	?	1
46	?	6	TYR	C	175.792	?	1
47	?	6	TYR	H	8.090	?	1
48	?	6	TYR	HA	4.662	?	1
49	?	6	TYR	HB2	3.017	?	2
50	?	6	TYR	HB3	2.837	?	2
51	?	6	TYR	HD1	7.103	?	3
52	?	6	TYR	HD2	7.103	?	3
53	?	6	TYR	HE1	6.782	?	3
54	?	6	TYR	HE2	6.782	?	3
55	?	6	TYR	CA	57.935	?	1
56	?	6	TYR	CB	38.789	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
57	?	6	TYR	CD1	133.282	?	3
58	?	6	TYR	CD2	133.282	?	3
59	?	6	TYR	CE1	118.277	?	3
60	?	6	TYR	CE2	118.277	?	3
61	?	6	TYR	N	121.327	?	1
62	?	7	THR	C	173.663	?	1
63	?	7	THR	H	8.043	?	1
64	?	7	THR	HA	4.292	?	1
65	?	7	THR	HB	4.152	?	1
66	?	7	THR	HG21	1.150	?	1
67	?	7	THR	HG22	1.150	?	1
68	?	7	THR	HG23	1.150	?	1
69	?	7	THR	CA	61.789	?	1
70	?	7	THR	CB	69.814	?	1
71	?	7	THR	CG2	21.496	?	1
72	?	7	THR	N	115.574	?	1
73	?	8	ASN	C	175.118	?	1
74	?	8	ASN	H	8.285	?	1
75	?	8	ASN	HA	4.744	?	1
76	?	8	ASN	HB2	2.839	?	2
77	?	8	ASN	HB3	2.772	?	2
78	?	8	ASN	CA	53.205	?	1
79	?	8	ASN	CB	38.897	?	1
80	?	8	ASN	N	120.533	?	1
81	?	9	LEU	C	177.017	?	1
82	?	9	LEU	H	8.111	?	1
83	?	9	LEU	HA	4.347	?	1
84	?	9	LEU	CA	55.651	?	1
85	?	9	LEU	CB	42.477	?	1
86	?	9	LEU	CG	27.039	?	1
87	?	9	LEU	CD1	23.429	?	2
88	?	9	LEU	CD2	25.234	?	2
89	?	9	LEU	N	122.112	?	1
90	?	10	LYS	C	176.507	?	1
91	?	10	LYS	H	8.137	?	1
92	?	10	LYS	HA	4.429	?	1
93	?	10	LYS	HB2	1.705	?	2
94	?	10	LYS	HB3	1.873	?	2
95	?	10	LYS	HG2	1.405	?	2
96	?	10	LYS	HG3	1.678	?	2
97	?	10	LYS	HE2	3.009	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
98	?	10	LYS	HE3	3.009	?	2
99	?	10	LYS	CA	55.320	?	1
100	?	10	LYS	CB	33.068	?	1
101	?	10	LYS	CG	24.813	?	1
102	?	10	LYS	CD	28.861	?	1
103	?	10	LYS	CE	42.190	?	1
104	?	10	LYS	N	119.034	?	1
105	?	11	CYS	H	8.269	?	1
106	?	11	CYS	HA	4.551	?	1
107	?	11	CYS	HB2	3.929	?	2
108	?	11	CYS	HB3	2.635	?	2
109	?	11	CYS	CA	54.826	?	1
110	?	11	CYS	CB	38.997	?	1
111	?	11	CYS	N	119.269	?	1
112	?	12	ARG	H	11.301	?	1
113	?	12	ARG	HA	4.221	?	1
114	?	12	ARG	HB2	1.744	?	2
115	?	12	ARG	HB3	1.799	?	2
116	?	12	ARG	HG2	1.631	?	2
117	?	12	ARG	HG3	1.647	?	2
118	?	12	ARG	HD2	3.098	?	2
119	?	12	ARG	HD3	3.094	?	2
120	?	12	ARG	CA	57.671	?	1
121	?	12	ARG	CB	31.744	?	1
122	?	12	ARG	CG	27.421	?	1
123	?	12	ARG	CD	43.634	?	1
124	?	12	ARG	N	127.141	?	1
125	?	13	CYS	H	9.397	?	1
126	?	13	CYS	HA	4.747	?	1
127	?	13	CYS	HB2	2.965	?	2
128	?	13	CYS	HB3	3.151	?	2
129	?	13	CYS	CA	54.667	?	1
130	?	13	CYS	CB	42.865	?	1
131	?	13	CYS	N	120.183	?	1
132	?	14	SER	H	8.757	?	1
133	?	14	SER	HA	4.412	?	1
134	?	14	SER	CA	58.612	?	1
135	?	14	SER	CB	63.069	?	1
136	?	14	SER	N	119.870	?	1
137	?	15	GLY	H	7.905	?	1
138	?	15	GLY	HA2	3.892	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
139	?	15	GLY	HA3	4.012	?	2
140	?	15	GLY	CA	44.752	?	1
141	?	15	GLY	N	110.733	?	1
142	?	16	VAL	H	8.122	?	1
143	?	16	VAL	HA	4.488	?	1
144	?	16	VAL	HB	1.878	?	1
145	?	16	VAL	HG11	0.772	?	1
146	?	16	VAL	HG12	0.772	?	1
147	?	16	VAL	HG13	0.772	?	1
148	?	16	VAL	HG21	0.779	?	1
149	?	16	VAL	HG22	0.779	?	1
150	?	16	VAL	HG23	0.779	?	1
151	?	16	VAL	CA	60.049	?	1
152	?	16	VAL	CB	34.827	?	1
153	?	16	VAL	CG1	22.001	?	1
154	?	16	VAL	CG2	19.249	?	1
155	?	16	VAL	N	114.774	?	1
156	?	17	ILE	H	8.441	?	1
157	?	17	ILE	HA	4.549	?	1
158	?	17	ILE	HB	1.969	?	1
159	?	17	ILE	HG12	1.300	?	2
160	?	17	ILE	HG13	1.482	?	2
161	?	17	ILE	HG21	0.962	?	1
162	?	17	ILE	HG22	0.962	?	1
163	?	17	ILE	HG23	0.962	?	1
164	?	17	ILE	HD11	0.790	?	1
165	?	17	ILE	HD12	0.790	?	1
166	?	17	ILE	HD13	0.790	?	1
167	?	17	ILE	CA	60.240	?	1
168	?	17	ILE	CB	39.981	?	1
169	?	17	ILE	CG1	26.863	?	1
170	?	17	ILE	CG2	18.119	?	1
171	?	17	ILE	CD1	13.421	?	1
172	?	17	ILE	N	121.144	?	1
173	?	18	SER	H	9.077	?	1
174	?	18	SER	HA	4.779	?	1
175	?	18	SER	HB2	3.955	?	2
176	?	18	SER	HB3	3.955	?	2
177	?	18	SER	CA	58.727	?	1
178	?	18	SER	CB	64.447	?	1
179	?	18	SER	N	118.780	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
180	?	19	THR	H	7.427	?	1
181	?	19	THR	HA	4.236	?	1
182	?	19	THR	HB	4.055	?	1
183	?	19	THR	HG21	1.140	?	1
184	?	19	THR	HG22	1.140	?	1
185	?	19	THR	HG23	1.140	?	1
186	?	19	THR	CA	61.345	?	1
187	?	19	THR	CB	69.936	?	1
188	?	19	THR	CG2	21.664	?	1
189	?	19	THR	N	116.210	?	1
190	?	20	VAL	H	7.656	?	1
191	?	20	VAL	HA	2.091	?	1
192	?	20	VAL	HB	1.348	?	1
193	?	20	VAL	HG11	0.220	?	1
194	?	20	VAL	HG12	0.220	?	1
195	?	20	VAL	HG13	0.220	?	1
196	?	20	VAL	HG21	0.419	?	1
197	?	20	VAL	HG22	0.419	?	1
198	?	20	VAL	HG23	0.419	?	1
199	?	20	VAL	CA	62.753	?	1
200	?	20	VAL	CB	32.256	?	1
201	?	20	VAL	CG1	20.241	?	1
202	?	20	VAL	CG2	20.868	?	1
203	?	20	VAL	N	120.206	?	1
204	?	21	VAL	H	5.205	?	1
205	?	21	VAL	HA	3.795	?	1
206	?	21	VAL	HB	1.626	?	1
207	?	21	VAL	HG11	0.671	?	1
208	?	21	VAL	HG12	0.671	?	1
209	?	21	VAL	HG13	0.671	?	1
210	?	21	VAL	HG21	0.717	?	1
211	?	21	VAL	HG22	0.717	?	1
212	?	21	VAL	HG23	0.717	?	1
213	?	21	VAL	CA	60.847	?	1
214	?	21	VAL	CB	33.521	?	1
215	?	21	VAL	CG1	20.998	?	1
216	?	21	VAL	CG2	21.228	?	1
217	?	22	GLY	H	8.154	?	1
218	?	22	GLY	HA2	3.542	?	2
219	?	22	GLY	HA3	3.812	?	2
220	?	22	GLY	CA	45.144	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
221	?	22	GLY	N	112.123	?	1
222	?	23	LEU	H	8.170	?	1
223	?	23	LEU	HA	3.849	?	1
224	?	23	LEU	HB2	1.540	?	2
225	?	23	LEU	HB3	1.586	?	2
226	?	23	LEU	HG	1.682	?	1
227	?	23	LEU	HD11	0.883	?	1
228	?	23	LEU	HD12	0.883	?	1
229	?	23	LEU	HD13	0.883	?	1
230	?	23	LEU	HD21	0.837	?	1
231	?	23	LEU	HD22	0.837	?	1
232	?	23	LEU	HD23	0.837	?	1
233	?	23	LEU	CA	57.689	?	1
234	?	23	LEU	CB	41.774	?	1
235	?	23	LEU	CG	27.164	?	1
236	?	23	LEU	CD1	24.450	?	1
237	?	23	LEU	CD2	24.669	?	1
238	?	23	LEU	N	122.616	?	1
239	?	24	ASN	H	8.463	?	1
240	?	24	ASN	HA	4.382	?	1
241	?	24	ASN	HB2	2.753	?	2
242	?	24	ASN	HB3	2.840	?	2
243	?	24	ASN	CA	55.137	?	1
244	?	24	ASN	CB	37.257	?	1
245	?	24	ASN	N	112.984	?	1
246	?	25	ILE	H	7.343	?	1
247	?	25	ILE	HA	4.482	?	1
248	?	25	ILE	HB	2.193	?	1
249	?	25	ILE	HG12	1.150	?	2
250	?	25	ILE	HG13	1.297	?	2
251	?	25	ILE	HG21	0.833	?	1
252	?	25	ILE	HG22	0.833	?	1
253	?	25	ILE	HG23	0.833	?	1
254	?	25	ILE	HD11	0.829	?	1
255	?	25	ILE	HD12	0.829	?	1
256	?	25	ILE	HD13	0.829	?	1
257	?	25	ILE	CA	60.597	?	1
258	?	25	ILE	CB	39.238	?	1
259	?	25	ILE	CG1	26.883	?	1
260	?	25	ILE	CG2	17.798	?	1
261	?	25	ILE	CD1	14.555	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
262	?	25	ILE	N	112.775	?	1
263	?	26	ILE	H	7.339	?	1
264	?	26	ILE	HA	3.499	?	1
265	?	26	ILE	HB	1.903	?	1
266	?	26	ILE	HG12	1.997	?	2
267	?	26	ILE	HG13	0.693	?	2
268	?	26	ILE	HG21	0.740	?	1
269	?	26	ILE	HG22	0.740	?	1
270	?	26	ILE	HG23	0.740	?	1
271	?	26	ILE	HD11	0.816	?	1
272	?	26	ILE	HD12	0.816	?	1
273	?	26	ILE	HD13	0.816	?	1
274	?	26	ILE	CA	64.301	?	1
275	?	26	ILE	CB	39.291	?	1
276	?	26	ILE	CG1	28.115	?	1
277	?	26	ILE	CG2	16.816	?	1
278	?	26	ILE	CD1	14.573	?	1
279	?	26	ILE	N	123.170	?	1
280	?	27	ASP	H	9.053	?	1
281	?	27	ASP	HA	4.892	?	1
282	?	27	ASP	HB2	2.161	?	2
283	?	27	ASP	HB3	2.583	?	2
284	?	27	ASP	CA	55.460	?	1
285	?	27	ASP	CB	43.766	?	1
286	?	27	ASP	N	127.762	?	1
287	?	28	ARG	H	7.901	?	1
288	?	28	ARG	HA	4.691	?	1
289	?	28	ARG	HB2	1.728	?	2
290	?	28	ARG	HB3	1.730	?	2
291	?	28	ARG	HG2	1.405	?	2
292	?	28	ARG	HG3	1.406	?	2
293	?	28	ARG	HD2	2.672	?	2
294	?	28	ARG	HD3	2.681	?	2
295	?	28	ARG	CA	55.039	?	1
296	?	28	ARG	CB	33.809	?	1
297	?	28	ARG	CG	26.942	?	1
298	?	28	ARG	CD	43.151	?	1
299	?	28	ARG	N	114.365	?	1
300	?	29	ILE	H	8.647	?	1
301	?	29	ILE	HA	5.135	?	1
302	?	29	ILE	HB	1.607	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
303	?	29	ILE	HG12	1.588	?	2
304	?	29	ILE	HG13	0.870	?	2
305	?	29	ILE	HG21	0.743	?	1
306	?	29	ILE	HG22	0.743	?	1
307	?	29	ILE	HG23	0.743	?	1
308	?	29	ILE	HD11	0.760	?	1
309	?	29	ILE	HD12	0.760	?	1
310	?	29	ILE	HD13	0.760	?	1
311	?	29	ILE	CA	60.359	?	1
312	?	29	ILE	CB	41.315	?	1
313	?	29	ILE	CG1	28.083	?	1
314	?	29	ILE	CG2	16.827	?	1
315	?	29	ILE	CD1	14.528	?	1
316	?	29	ILE	N	121.462	?	1
317	?	30	GLN	H	9.544	?	1
318	?	30	GLN	HA	4.784	?	1
319	?	30	GLN	HB2	2.025	?	2
320	?	30	GLN	HB3	2.284	?	2
321	?	30	GLN	HG2	2.228	?	2
322	?	30	GLN	HG3	2.297	?	2
323	?	30	GLN	CA	55.040	?	1
324	?	30	GLN	CB	33.039	?	1
325	?	30	GLN	CG	34.071	?	1
326	?	30	GLN	N	127.865	?	1
327	?	31	VAL	H	8.900	?	1
328	?	31	VAL	HA	4.764	?	1
329	?	31	VAL	HB	1.982	?	1
330	?	31	VAL	HG11	0.741	?	1
331	?	31	VAL	HG12	0.741	?	1
332	?	31	VAL	HG13	0.741	?	1
333	?	31	VAL	HG21	0.888	?	1
334	?	31	VAL	HG22	0.888	?	1
335	?	31	VAL	HG23	0.888	?	1
336	?	31	VAL	CA	61.561	?	1
337	?	31	VAL	CB	32.989	?	1
338	?	31	VAL	CG1	20.797	?	1
339	?	31	VAL	CG2	21.392	?	1
340	?	31	VAL	N	128.831	?	1
341	?	32	THR	H	9.383	?	1
342	?	32	THR	HA	4.930	?	1
343	?	32	THR	HB	4.118	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
344	?	32	THR	HG21	1.322	?	1
345	?	32	THR	HG22	1.322	?	1
346	?	32	THR	HG23	1.322	?	1
347	?	32	THR	CA	58.787	?	1
348	?	32	THR	CB	70.306	?	1
349	?	32	THR	CG2	21.860	?	1
350	?	32	THR	N	125.430	?	1
351	?	33	PRO	HA	4.763	?	1
352	?	33	PRO	HB2	1.926	?	2
353	?	34	PRO	HA	4.394	?	1
354	?	34	PRO	HB2	1.840	?	2
355	?	34	PRO	HB3	1.721	?	2
356	?	34	PRO	HG2	1.663	?	2
357	?	34	PRO	HG3	1.894	?	2
358	?	34	PRO	HD2	3.383	?	2
359	?	34	PRO	HD3	3.888	?	2
360	?	34	PRO	CA	63.105	?	1
361	?	34	PRO	CB	32.349	?	1
362	?	34	PRO	CG	27.549	?	1
363	?	34	PRO	CD	49.849	?	1
364	?	35	GLY	H	8.298	?	1
365	?	35	GLY	HA2	3.915	?	2
366	?	35	GLY	HA3	4.178	?	2
367	?	35	GLY	CA	44.993	?	1
368	?	35	GLY	N	109.067	?	1
369	?	36	ASN	H	8.895	?	1
370	?	36	ASN	HA	4.464	?	1
371	?	36	ASN	HB2	2.662	?	2
372	?	36	ASN	HB3	2.888	?	2
373	?	36	ASN	CA	54.352	?	1
374	?	36	ASN	CB	38.267	?	1
375	?	36	ASN	N	118.981	?	1
376	?	37	GLY	H	8.374	?	1
377	?	37	GLY	HA2	3.613	?	2
378	?	37	GLY	HA3	4.216	?	2
379	?	37	GLY	CA	45.475	?	1
380	?	37	GLY	N	107.259	?	1
381	?	38	CYS	H	7.713	?	1
382	?	38	CYS	HA	5.315	?	1
383	?	38	CYS	HB2	2.749	?	2
384	?	38	CYS	HB3	3.326	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
385	?	38	CYS	CA	52.336	?	1
386	?	38	CYS	CB	41.831	?	1
387	?	38	CYS	N	119.609	?	1
388	?	39	PRO	HA	4.700	?	1
389	?	39	PRO	HB2	2.109	?	2
390	?	39	PRO	HB3	2.218	?	2
391	?	39	PRO	HG2	1.788	?	2
392	?	39	PRO	HG3	2.053	?	2
393	?	39	PRO	HD2	3.914	?	2
394	?	39	PRO	HD3	3.956	?	2
395	?	39	PRO	CA	63.817	?	1
396	?	39	PRO	CB	31.415	?	1
397	?	39	PRO	CG	26.816	?	1
398	?	39	PRO	CD	51.190	?	1
399	?	40	LYS	H	7.410	?	1
400	?	40	LYS	HA	4.673	?	1
401	?	40	LYS	HB2	1.617	?	2
402	?	40	LYS	HB3	1.779	?	2
403	?	40	LYS	HG2	1.196	?	2
404	?	40	LYS	HG3	1.292	?	2
405	?	40	LYS	HD2	1.603	?	2
406	?	40	LYS	HD3	1.611	?	2
407	?	40	LYS	HE2	2.958	?	2
408	?	40	LYS	CA	54.480	?	1
409	?	40	LYS	CB	35.512	?	1
410	?	40	LYS	CG	24.435	?	1
411	?	40	LYS	CD	29.426	?	1
412	?	40	LYS	CE	42.527	?	1
413	?	40	LYS	N	119.155	?	1
414	?	41	THR	H	8.325	?	1
415	?	41	THR	HA	4.425	?	1
416	?	41	THR	HB	3.802	?	1
417	?	41	THR	HG21	0.966	?	1
418	?	41	THR	HG22	0.966	?	1
419	?	41	THR	HG23	0.966	?	1
420	?	41	THR	CA	63.648	?	1
421	?	41	THR	CB	69.192	?	1
422	?	41	THR	CG2	21.510	?	1
423	?	41	THR	N	119.584	?	1
424	?	42	GLU	H	8.511	?	1
425	?	42	GLU	HA	4.691	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
426	?	42	GLU	HB2	1.735	?	2
427	?	42	GLU	HB3	1.997	?	2
428	?	42	GLU	HG2	1.769	?	2
429	?	42	GLU	HG3	2.302	?	2
430	?	42	GLU	CA	55.806	?	1
431	?	42	GLU	CB	33.029	?	1
432	?	42	GLU	CG	38.974	?	1
433	?	42	GLU	N	124.520	?	1
434	?	43	VAL	H	9.243	?	1
435	?	43	VAL	HA	4.684	?	1
436	?	43	VAL	HB	1.971	?	1
437	?	43	VAL	HG11	0.657	?	1
438	?	43	VAL	HG12	0.657	?	1
439	?	43	VAL	HG13	0.657	?	1
440	?	43	VAL	HG21	0.791	?	1
441	?	43	VAL	HG22	0.791	?	1
442	?	43	VAL	HG23	0.791	?	1
443	?	43	VAL	CA	61.849	?	1
444	?	43	VAL	CB	32.658	?	1
445	?	43	VAL	CG1	21.220	?	1
446	?	43	VAL	CG2	21.303	?	1
447	?	43	VAL	N	124.960	?	1
448	?	44	VAL	H	8.666	?	1
449	?	44	VAL	HA	4.610	?	1
450	?	44	VAL	HB	1.710	?	1
451	?	44	VAL	HG11	0.108	?	1
452	?	44	VAL	HG12	0.108	?	1
453	?	44	VAL	HG13	0.108	?	1
454	?	44	VAL	HG21	0.720	?	1
455	?	44	VAL	HG22	0.720	?	1
456	?	44	VAL	HG23	0.720	?	1
457	?	44	VAL	CA	60.545	?	1
458	?	44	VAL	CB	34.525	?	1
459	?	44	VAL	CG1	21.724	?	1
460	?	44	VAL	CG2	21.269	?	1
461	?	44	VAL	N	126.067	?	1
462	?	45	ILE	H	9.087	?	1
463	?	45	ILE	HA	4.826	?	1
464	?	45	ILE	HB	1.745	?	1
465	?	45	ILE	HG12	1.604	?	2
466	?	45	ILE	HG13	1.599	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
467	?	45	ILE	HG21	0.818	?	1
468	?	45	ILE	HG22	0.818	?	1
469	?	45	ILE	HG23	0.818	?	1
470	?	45	ILE	HD11	0.834	?	1
471	?	45	ILE	HD12	0.834	?	1
472	?	45	ILE	HD13	0.834	?	1
473	?	45	ILE	CA	59.908	?	1
474	?	45	ILE	CB	41.077	?	1
475	?	45	ILE	CG1	28.459	?	1
476	?	45	ILE	CG2	18.463	?	1
477	?	45	ILE	CD1	14.487	?	1
478	?	45	ILE	N	124.729	?	1
479	?	46	TRP	H	9.022	?	1
480	?	46	TRP	HA	5.277	?	1
481	?	46	TRP	HB2	3.110	?	2
482	?	46	TRP	HB3	3.303	?	2
483	?	46	TRP	HD1	6.985	?	1
484	?	46	TRP	HE1	9.931	?	1
485	?	46	TRP	HE3	7.423	?	1
486	?	46	TRP	HZ2	7.299	?	1
487	?	46	TRP	HZ3	6.859	?	1
488	?	46	TRP	HH2	6.997	?	1
489	?	46	TRP	CA	56.886	?	1
490	?	46	TRP	CB	31.167	?	1
491	?	46	TRP	CD1	126.513	?	1
492	?	46	TRP	CE3	121.906	?	1
493	?	46	TRP	CZ2	114.190	?	1
494	?	46	TRP	CZ3	121.402	?	1
495	?	46	TRP	CH2	124.028	?	1
496	?	46	TRP	N	127.530	?	1
497	?	46	TRP	NE1	128.701	?	1
498	?	47	THR	H	9.266	?	1
499	?	47	THR	HA	5.234	?	1
500	?	47	THR	HB	4.776	?	1
501	?	47	THR	HG1	5.836	?	1
502	?	47	THR	HG21	1.094	?	1
503	?	47	THR	HG22	1.094	?	1
504	?	47	THR	HG23	1.094	?	1
505	?	47	THR	CA	59.995	?	1
506	?	47	THR	CB	72.111	?	1
507	?	47	THR	CG2	21.581	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
508	?	47	THR	N	114.664	?	1
509	?	48	LYS	H	8.983	?	1
510	?	48	LYS	HA	4.155	?	1
511	?	48	LYS	HB2	1.701	?	2
512	?	48	LYS	HB3	2.025	?	2
513	?	48	LYS	HG2	1.237	?	2
514	?	48	LYS	HG3	1.385	?	2
515	?	48	LYS	HD2	1.670	?	2
516	?	48	LYS	HD3	1.674	?	2
517	?	48	LYS	HE2	2.901	?	2
518	?	48	LYS	HE3	2.900	?	2
519	?	48	LYS	CA	58.936	?	1
520	?	48	LYS	CB	32.581	?	1
521	?	48	LYS	CG	26.544	?	1
522	?	48	LYS	CD	29.453	?	1
523	?	48	LYS	CE	42.498	?	1
524	?	48	LYS	N	121.475	?	1
525	?	49	MET	H	7.617	?	1
526	?	49	MET	HA	4.649	?	1
527	?	49	MET	HB2	1.789	?	2
528	?	49	MET	HB3	2.351	?	2
529	?	49	MET	HG2	2.537	?	2
530	?	49	MET	HG3	2.645	?	2
531	?	49	MET	HE1	2.061	?	1
532	?	49	MET	HE2	2.061	?	1
533	?	49	MET	HE3	2.061	?	1
534	?	49	MET	CA	55.064	?	1
535	?	49	MET	CB	30.922	?	1
536	?	49	MET	CG	33.284	?	1
537	?	49	MET	CE	17.378	?	1
538	?	49	MET	N	116.227	?	1
539	?	50	LYS	H	8.073	?	1
540	?	50	LYS	HA	3.851	?	1
541	?	50	LYS	HB2	2.014	?	2
542	?	50	LYS	HB3	2.181	?	2
543	?	50	LYS	HG2	1.327	?	2
544	?	50	LYS	HG3	1.328	?	2
545	?	50	LYS	HD2	1.657	?	2
546	?	50	LYS	HD3	1.651	?	2
547	?	50	LYS	HE2	2.974	?	2
548	?	50	LYS	HE3	2.971	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
549	?	50	LYS	CA	57.628	?	1
550	?	50	LYS	CB	28.426	?	1
551	?	50	LYS	CG	25.265	?	1
552	?	50	LYS	CD	29.165	?	1
553	?	50	LYS	CE	42.449	?	1
554	?	50	LYS	N	113.319	?	1
555	?	51	LYS	H	7.162	?	1
556	?	51	LYS	HA	4.533	?	1
557	?	51	LYS	HB2	1.643	?	2
558	?	51	LYS	HB3	1.632	?	2
559	?	51	LYS	HG2	1.168	?	2
560	?	51	LYS	HG3	1.326	?	2
561	?	51	LYS	HD2	1.587	?	2
562	?	51	LYS	HD3	1.591	?	2
563	?	51	LYS	HE2	2.899	?	2
564	?	51	LYS	HE3	2.898	?	2
565	?	51	LYS	CA	54.628	?	1
566	?	51	LYS	CB	33.767	?	1
567	?	51	LYS	CG	25.031	?	1
568	?	51	LYS	CD	28.681	?	1
569	?	51	LYS	CE	42.380	?	1
570	?	51	LYS	N	117.452	?	1
571	?	52	VAL	H	8.094	?	1
572	?	52	VAL	HA	4.521	?	1
573	?	52	VAL	HB	1.448	?	1
574	?	52	VAL	HG11	0.146	?	1
575	?	52	VAL	HG12	0.146	?	1
576	?	52	VAL	HG13	0.146	?	1
577	?	52	VAL	HG21	0.262	?	1
578	?	52	VAL	HG22	0.262	?	1
579	?	52	VAL	HG23	0.262	?	1
580	?	52	VAL	CA	61.297	?	1
581	?	52	VAL	CB	32.820	?	1
582	?	52	VAL	CG1	20.659	?	1
583	?	52	VAL	CG2	20.561	?	1
584	?	52	VAL	N	122.544	?	1
585	?	53	ILE	H	9.110	?	1
586	?	53	ILE	HA	4.305	?	1
587	?	53	ILE	HB	1.593	?	1
588	?	53	ILE	HG12	0.895	?	2
589	?	53	ILE	HG13	1.279	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
590	?	53	ILE	HG21	0.748	?	1
591	?	53	ILE	HG22	0.748	?	1
592	?	53	ILE	HG23	0.748	?	1
593	?	53	ILE	HD11	0.635	?	1
594	?	53	ILE	HD12	0.635	?	1
595	?	53	ILE	HD13	0.635	?	1
596	?	53	ILE	CA	59.977	?	1
597	?	53	ILE	CB	41.975	?	1
598	?	53	ILE	CG1	26.716	?	1
599	?	53	ILE	CG2	17.785	?	1
600	?	53	ILE	CD1	13.910	?	1
601	?	53	ILE	N	126.275	?	1
602	?	54	CYS	H	8.621	?	1
603	?	54	CYS	HA	5.469	?	1
604	?	54	CYS	HB2	3.067	?	2
605	?	54	CYS	HB3	3.783	?	2
606	?	54	CYS	CA	57.120	?	1
607	?	54	CYS	CB	47.633	?	1
608	?	54	CYS	N	123.413	?	1
609	?	55	VAL	H	8.262	?	1
610	?	55	VAL	HA	4.845	?	1
611	?	55	VAL	HB	1.882	?	1
612	?	55	VAL	HG11	0.924	?	1
613	?	55	VAL	HG12	0.924	?	1
614	?	55	VAL	HG13	0.924	?	1
615	?	55	VAL	HG21	0.770	?	1
616	?	55	VAL	HG22	0.770	?	1
617	?	55	VAL	HG23	0.770	?	1
618	?	55	VAL	CA	59.807	?	1
619	?	55	VAL	CB	35.000	?	1
620	?	55	VAL	CG1	22.473	?	1
621	?	55	VAL	CG2	21.062	?	1
622	?	55	VAL	N	117.865	?	1
623	?	56	ASN	H	8.411	?	1
624	?	56	ASN	HA	4.472	?	1
625	?	56	ASN	HB2	2.695	?	2
626	?	56	ASN	HB3	2.870	?	2
627	?	56	ASN	CA	50.964	?	1
628	?	56	ASN	CB	39.456	?	1
629	?	56	ASN	N	124.058	?	1
630	?	57	PRO	HA	3.946	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
631	?	57	PRO	HB2	1.807	?	2
632	?	57	PRO	HB3	2.005	?	2
633	?	57	PRO	HG2	1.875	?	2
634	?	57	PRO	HG3	1.867	?	2
635	?	57	PRO	HD2	3.740	?	2
636	?	57	PRO	HD3	4.171	?	2
637	?	57	PRO	CA	64.105	?	1
638	?	57	PRO	CB	32.395	?	1
639	?	57	PRO	CG	27.664	?	1
640	?	57	PRO	CD	51.298	?	1
641	?	58	ARG	H	7.745	?	1
642	?	58	ARG	HA	4.112	?	1
643	?	58	ARG	HB2	1.532	?	2
644	?	58	ARG	HB3	1.951	?	2
645	?	58	ARG	HG2	1.510	?	2
646	?	58	ARG	HG3	1.520	?	2
647	?	58	ARG	HD2	3.130	?	2
648	?	58	ARG	HD3	3.121	?	2
649	?	58	ARG	CA	54.892	?	1
650	?	58	ARG	CB	29.911	?	1
651	?	58	ARG	CG	27.577	?	1
652	?	58	ARG	CD	43.249	?	1
653	?	58	ARG	N	113.096	?	1
654	?	59	ALA	H	7.550	?	1
655	?	59	ALA	HA	4.084	?	1
656	?	59	ALA	HB1	0.974	?	1
657	?	59	ALA	HB2	0.974	?	1
658	?	59	ALA	HB3	0.974	?	1
659	?	59	ALA	CA	52.868	?	1
660	?	59	ALA	CB	18.017	?	1
661	?	59	ALA	N	124.131	?	1
662	?	60	LYS	H	8.999	?	1
663	?	60	LYS	HA	3.877	?	1
664	?	60	LYS	HB2	1.877	?	2
665	?	60	LYS	HB3	1.955	?	2
666	?	60	LYS	HG2	1.467	?	2
667	?	60	LYS	HG3	1.573	?	2
668	?	60	LYS	HD2	1.694	?	2
669	?	60	LYS	HD3	1.699	?	2
670	?	60	LYS	HE2	2.992	?	2
671	?	60	LYS	HE3	2.992	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
672	?	60	LYS	CA	59.898	?	1
673	?	60	LYS	CB	31.823	?	1
674	?	60	LYS	CG	25.381	?	1
675	?	60	LYS	CD	29.138	?	1
676	?	60	LYS	CE	42.141	?	1
677	?	60	LYS	N	126.126	?	1
678	?	61	TRP	H	7.761	?	1
679	?	61	TRP	HA	4.368	?	1
680	?	61	TRP	HB2	3.234	?	2
681	?	61	TRP	HB3	3.518	?	2
682	?	61	TRP	HD1	7.610	?	1
683	?	61	TRP	HE1	10.026	?	1
684	?	61	TRP	HE3	7.309	?	1
685	?	61	TRP	HZ2	7.358	?	1
686	?	61	TRP	HZ3	6.873	?	1
687	?	61	TRP	HH2	6.860	?	1
688	?	61	TRP	CA	57.431	?	1
689	?	61	TRP	CB	27.594	?	1
690	?	61	TRP	CD1	128.542	?	1
691	?	61	TRP	CE3	120.545	?	1
692	?	61	TRP	CZ2	115.361	?	1
693	?	61	TRP	CZ3	122.786	?	1
694	?	61	TRP	CH2	123.923	?	1
695	?	61	TRP	N	115.958	?	1
696	?	61	TRP	NE1	130.887	?	1
697	?	62	LEU	H	5.882	?	1
698	?	62	LEU	HA	3.528	?	1
699	?	62	LEU	HB2	0.037	?	2
700	?	62	LEU	HB3	1.239	?	2
701	?	62	LEU	HG	1.060	?	1
702	?	62	LEU	HD11	0.533	?	1
703	?	62	LEU	HD12	0.533	?	1
704	?	62	LEU	HD13	0.533	?	1
705	?	62	LEU	HD21	0.525	?	1
706	?	62	LEU	HD22	0.525	?	1
707	?	62	LEU	HD23	0.525	?	1
708	?	62	LEU	CA	56.399	?	1
709	?	62	LEU	CB	41.658	?	1
710	?	62	LEU	CG	26.395	?	1
711	?	62	LEU	CD1	23.448	?	1
712	?	62	LEU	CD2	25.315	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
713	?	62	LEU	N	123.199	?	1
714	?	63	GLN	H	7.528	?	1
715	?	63	GLN	HA	3.694	?	1
716	?	63	GLN	HB2	2.007	?	2
717	?	63	GLN	HB3	2.081	?	2
718	?	63	GLN	HG2	2.317	?	2
719	?	63	GLN	HG3	2.371	?	2
720	?	63	GLN	CA	59.198	?	1
721	?	63	GLN	CB	27.897	?	1
722	?	63	GLN	CG	33.704	?	1
723	?	63	GLN	N	117.164	?	1
724	?	64	ARG	H	7.847	?	1
725	?	64	ARG	HA	4.008	?	1
726	?	64	ARG	HB2	1.889	?	2
727	?	64	ARG	HB3	1.891	?	2
728	?	64	ARG	HG2	1.627	?	2
729	?	64	ARG	HG3	1.715	?	2
730	?	64	ARG	HD2	3.229	?	2
731	?	64	ARG	HD3	3.228	?	2
732	?	64	ARG	CA	59.155	?	1
733	?	64	ARG	CB	30.108	?	1
734	?	64	ARG	CG	27.615	?	1
735	?	64	ARG	CD	43.578	?	1
736	?	64	ARG	N	116.909	?	1
737	?	65	LEU	H	7.475	?	1
738	?	65	LEU	HA	4.215	?	1
739	?	65	LEU	HB2	1.744	?	2
740	?	65	LEU	HB3	1.883	?	2
741	?	65	LEU	HG	1.755	?	1
742	?	65	LEU	HD11	1.036	?	1
743	?	65	LEU	HD12	1.036	?	1
744	?	65	LEU	HD13	1.036	?	1
745	?	65	LEU	HD21	0.918	?	1
746	?	65	LEU	HD22	0.918	?	1
747	?	65	LEU	HD23	0.918	?	1
748	?	65	LEU	CA	57.694	?	1
749	?	65	LEU	CB	42.242	?	1
750	?	65	LEU	CG	27.301	?	1
751	?	65	LEU	CD1	25.364	?	1
752	?	65	LEU	CD2	24.751	?	1
753	?	65	LEU	N	120.096	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
754	?	66	LEU	H	8.055	?	1
755	?	66	LEU	HA	4.019	?	1
756	?	66	LEU	HB2	1.437	?	2
757	?	66	LEU	HB3	1.692	?	2
758	?	66	LEU	HG	1.656	?	1
759	?	66	LEU	HD11	0.713	?	1
760	?	66	LEU	HD12	0.713	?	1
761	?	66	LEU	HD13	0.713	?	1
762	?	66	LEU	HD21	0.674	?	1
763	?	66	LEU	HD22	0.674	?	1
764	?	66	LEU	HD23	0.674	?	1
765	?	66	LEU	CA	56.973	?	1
766	?	66	LEU	CB	41.297	?	1
767	?	66	LEU	CG	26.720	?	1
768	?	66	LEU	CD1	25.423	?	1
769	?	66	LEU	CD2	22.586	?	1
770	?	66	LEU	N	117.426	?	1
771	?	67	ARG	H	7.572	?	1
772	?	67	ARG	HA	4.098	?	1
773	?	67	ARG	HB2	1.799	?	2
774	?	67	ARG	HB3	1.801	?	2
775	?	67	ARG	HG2	1.533	?	2
776	?	67	ARG	HG3	1.653	?	2
777	?	67	ARG	HD2	3.131	?	2
778	?	67	ARG	HD3	3.134	?	2
779	?	67	ARG	CA	57.988	?	1
780	?	67	ARG	CB	30.225	?	1
781	?	67	ARG	CG	27.458	?	1
782	?	67	ARG	CD	43.453	?	1
783	?	67	ARG	N	117.564	?	1
784	?	68	HIS	H	7.934	?	1
785	?	68	HIS	HA	4.553	?	1
786	?	68	HIS	HB2	3.179	?	2
787	?	68	HIS	HB3	3.313	?	2
788	?	68	HIS	HD2	7.085	?	1
789	?	68	HIS	HE1	8.073	?	1
790	?	68	HIS	CA	57.552	?	1
791	?	68	HIS	CB	30.294	?	1
792	?	68	HIS	CD2	120.137	?	1
793	?	68	HIS	CE1	137.834	?	1
794	?	68	HIS	N	118.270	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
795	?	69	VAL	H	8.003	?	1
796	?	69	VAL	HA	3.979	?	1
797	?	69	VAL	HB	2.129	?	1
798	?	69	VAL	HG11	0.918	?	2
799	?	69	VAL	HG12	0.918	?	2
800	?	69	VAL	HG13	0.918	?	2
801	?	69	VAL	HG21	0.955	?	2
802	?	69	VAL	HG22	0.955	?	2
803	?	69	VAL	HG23	0.955	?	2
804	?	69	VAL	CA	63.583	?	1
805	?	69	VAL	CB	32.290	?	1
806	?	69	VAL	CG1	20.826	?	2
807	?	69	VAL	CG2	21.242	?	2
808	?	69	VAL	N	118.941	?	1
809	?	70	GLN	H	8.275	?	1
810	?	70	GLN	HA	4.273	?	1
811	?	70	GLN	HB2	2.045	?	2
812	?	70	GLN	HB3	2.091	?	2
813	?	70	GLN	HG2	2.389	?	2
814	?	70	GLN	HG3	2.381	?	2
815	?	70	GLN	CA	56.601	?	1
816	?	70	GLN	CB	29.283	?	1
817	?	70	GLN	CG	34.040	?	1
818	?	70	GLN	N	122.062	?	1
819	?	71	SER	H	8.153	?	1
820	?	71	SER	HA	4.384	?	1
821	?	71	SER	HB2	3.862	?	2
822	?	71	SER	HB3	3.862	?	2
823	?	71	SER	CA	59.230	?	1
824	?	71	SER	CB	63.748	?	1
825	?	71	SER	N	116.298	?	1
826	?	72	LYS	H	8.156	?	1
827	?	72	LYS	HA	4.305	?	1
828	?	72	LYS	CA	56.542	?	1
829	?	72	LYS	CB	32.758	?	1
830	?	72	LYS	N	122.458	?	1
831	?	73	SER	H	8.161	?	1
832	?	73	SER	HA	4.424	?	1
833	?	73	SER	HB2	3.828	?	2
834	?	73	SER	HB3	3.828	?	2
835	?	73	SER	CA	58.571	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
836	?	73	SER	CB	63.772	?	1
837	?	73	SER	N	116.218	?	1
838	?	74	LEU	H	8.172	?	1
839	?	74	LEU	HA	4.372	?	1
840	?	74	LEU	HB2	1.600	?	2
841	?	74	LEU	HB3	1.601	?	2
842	?	74	LEU	HD11	0.860	?	1
843	?	74	LEU	HD12	0.860	?	1
844	?	74	LEU	HD13	0.860	?	1
845	?	74	LEU	HD21	0.814	?	1
846	?	74	LEU	HD22	0.814	?	1
847	?	74	LEU	HD23	0.814	?	1
848	?	74	LEU	CA	55.408	?	1
849	?	74	LEU	CB	42.365	?	1
850	?	74	LEU	CG	27.041	?	1
851	?	74	LEU	CD1	25.118	?	1
852	?	74	LEU	CD2	23.644	?	1
853	?	74	LEU	N	123.786	?	1
854	?	75	SER	H	8.188	?	1
855	?	75	SER	HA	4.434	?	1
856	?	75	SER	HB2	3.814	?	2
857	?	75	SER	HB3	3.814	?	2
858	?	75	SER	CA	58.272	?	1
859	?	75	SER	CB	63.949	?	1
860	?	75	SER	N	115.966	?	1
861	?	76	SER	H	8.240	?	1
862	?	76	SER	HA	4.476	?	1
863	?	76	SER	HB2	3.837	?	2
864	?	76	SER	HB3	3.841	?	2
865	?	76	SER	CA	58.215	?	1
866	?	76	SER	CB	63.954	?	1
867	?	76	SER	N	117.880	?	1
868	?	77	THR	H	8.129	?	1
869	?	77	THR	HA	4.564	?	1
870	?	77	THR	HB	4.091	?	1
871	?	77	THR	HG21	1.191	?	1
872	?	77	THR	HG22	1.191	?	1
873	?	77	THR	HG23	1.191	?	1
874	?	77	THR	CA	60.022	?	1
875	?	77	THR	CB	69.834	?	1
876	?	77	THR	CG2	21.463	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
877	?	77	THR	N	118.250	?	1
878	?	78	PRO	HA	4.364	?	1
879	?	78	PRO	HB2	1.846	?	2
880	?	78	PRO	HB3	2.244	?	2
881	?	78	PRO	HG2	1.984	?	2
882	?	78	PRO	HG3	1.956	?	2
883	?	78	PRO	HD2	3.651	?	2
884	?	78	PRO	HD3	3.813	?	2
885	?	78	PRO	CA	63.322	?	1
886	?	78	PRO	CB	32.150	?	1
887	?	78	PRO	CG	27.407	?	1
888	?	78	PRO	CD	51.194	?	1
889	?	79	GLN	H	8.415	?	1
890	?	79	GLN	HA	4.239	?	1
891	?	79	GLN	HB2	1.901	?	2
892	?	79	GLN	HB3	2.019	?	2
893	?	79	GLN	HG2	2.339	?	2
894	?	79	GLN	HG3	2.340	?	2
895	?	79	GLN	CA	55.487	?	1
896	?	79	GLN	CB	29.742	?	1
897	?	79	GLN	CG	33.882	?	1
898	?	79	GLN	N	120.979	?	1
899	?	80	ALA	H	8.292	?	1
900	?	80	ALA	HA	4.531	?	1
901	?	80	ALA	HB1	1.304	?	1
902	?	80	ALA	HB2	1.304	?	1
903	?	80	ALA	HB3	1.304	?	1
904	?	80	ALA	CA	50.540	?	1
905	?	80	ALA	CB	18.124	?	1
906	?	80	ALA	N	127.122	?	1
907	?	81	PRO	HA	4.412	?	1
908	?	81	PRO	HB2	1.848	?	2
909	?	81	PRO	HB3	2.242	?	2
910	?	81	PRO	HG2	1.972	?	2
911	?	81	PRO	HG3	1.976	?	2
912	?	81	PRO	HD2	3.589	?	2
913	?	81	PRO	HD3	3.755	?	2
914	?	81	PRO	CA	62.983	?	1
915	?	81	PRO	CB	32.073	?	1
916	?	81	PRO	CG	27.430	?	1
917	?	81	PRO	CD	50.553	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
918	?	82	VAL	H	8.204	?	1
919	?	82	VAL	HA	4.031	?	1
920	?	82	VAL	HB	2.015	?	1
921	?	82	VAL	HG11	0.906	?	2
922	?	82	VAL	HG12	0.906	?	2
923	?	82	VAL	HG13	0.906	?	2
924	?	82	VAL	HG21	0.909	?	2
925	?	82	VAL	HG22	0.909	?	2
926	?	82	VAL	HG23	0.909	?	2
927	?	82	VAL	CA	62.428	?	1
928	?	82	VAL	CB	32.754	?	1
929	?	82	VAL	CG1	21.057	?	2
930	?	82	VAL	CG2	20.864	?	2
931	?	82	VAL	N	120.446	?	1
932	?	83	SER	H	8.304	?	1
933	?	83	SER	HA	4.398	?	1
934	?	83	SER	HB2	3.798	?	2
935	?	83	SER	HB3	3.790	?	2
936	?	83	SER	CA	58.273	?	1
937	?	83	SER	CB	63.869	?	1
938	?	83	SER	N	119.326	?	1
939	?	84	LYS	H	8.303	?	1
940	?	84	LYS	HA	4.277	?	1
941	?	84	LYS	HB2	1.670	?	2
942	?	84	LYS	HB3	1.797	?	2
943	?	84	LYS	HG2	1.376	?	2
944	?	84	LYS	HG3	1.383	?	2
945	?	84	LYS	HD2	1.641	?	2
946	?	84	LYS	HD3	1.640	?	2
947	?	84	LYS	HE2	2.941	?	2
948	?	84	LYS	HE3	2.942	?	2
949	?	84	LYS	CA	56.363	?	1
950	?	84	LYS	CB	33.053	?	1
951	?	84	LYS	CG	24.753	?	1
952	?	84	LYS	CD	29.117	?	1
953	?	84	LYS	CE	42.193	?	1
954	?	84	LYS	N	123.696	?	1
955	?	85	ARG	H	8.236	?	1
956	?	85	ARG	HA	4.250	?	1
957	?	85	ARG	HB2	1.691	?	2
958	?	85	ARG	HB3	1.762	?	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
959	?	85	ARG	HG2	1.561	?	2
960	?	85	ARG	HG3	1.573	?	2
961	?	85	ARG	HD2	3.139	?	2
962	?	85	ARG	HD3	3.139	?	2
963	?	85	ARG	CA	56.084	?	1
964	?	85	ARG	CB	30.931	?	1
965	?	85	ARG	CG	27.112	?	1
966	?	85	ARG	CD	43.412	?	1
967	?	85	ARG	N	122.519	?	1
968	?	86	ARG	H	8.351	?	1
969	?	86	ARG	HA	4.256	?	1
970	?	86	ARG	HB2	1.699	?	2
971	?	86	ARG	HB3	1.788	?	2
972	?	86	ARG	HG2	1.586	?	2
973	?	86	ARG	HG3	1.587	?	2
974	?	86	ARG	HD2	3.152	?	2
975	?	86	ARG	HD3	3.152	?	2
976	?	86	ARG	CA	56.093	?	1
977	?	86	ARG	CB	30.991	?	1
978	?	86	ARG	CG	27.098	?	1
979	?	86	ARG	CD	43.433	?	1
980	?	86	ARG	N	123.332	?	1
981	?	87	ALA	H	8.316	?	1
982	?	87	ALA	HA	4.253	?	1
983	?	87	ALA	HB1	1.334	?	1
984	?	87	ALA	HB2	1.334	?	1
985	?	87	ALA	HB3	1.334	?	1
986	?	87	ALA	CA	52.448	?	1
987	?	87	ALA	CB	19.345	?	1
988	?	87	ALA	N	126.547	?	1
989	?	88	ALA	H	7.839	?	1
990	?	88	ALA	HA	4.044	?	1
991	?	88	ALA	HB1	1.272	?	1
992	?	88	ALA	HB2	1.272	?	1
993	?	88	ALA	HB3	1.272	?	1
994	?	88	ALA	CA	53.790	?	1
995	?	88	ALA	CB	20.146	?	1
996	?	88	ALA	N	128.957	?	1

### 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 743. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	0/282 (0%)	0/112 (0%)	0/116 (0%)	0/54 (0%)
Sidechain	0/429 (0%)	0/251 (0%)	0/155 (0%)	0/23 (0%)
Aromatic	0/32 (0%)	0/16 (0%)	0/12 (0%)	0/4 (0%)
Overall	0/743 (0%)	0/379 (0%)	0/283 (0%)	0/81 (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 1122. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	0/428 (0%)	0/170 (0%)	0/176 (0%)	0/82 (0%)
Sidechain	0/646 (0%)	0/381 (0%)	0/228 (0%)	0/37 (0%)
Aromatic	0/48 (0%)	0/24 (0%)	0/18 (0%)	0/6 (0%)
Overall	0/1122 (0%)	0/575 (0%)	0/422 (0%)	0/125 (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 (assigned\_chemical\_shifts). RCI is only applicable to proteins.