



Full wwPDB NMR Structure Validation Report ⓘ

Aug 30, 2017 – 08:13 PM EDT

PDB ID : 5J8T
Title : NMR structure of Excalibur domain of CbpL
Authors : Pantoja-Uceda, D.; Trevino, M.A.; Bruix, M.
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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-20029824
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

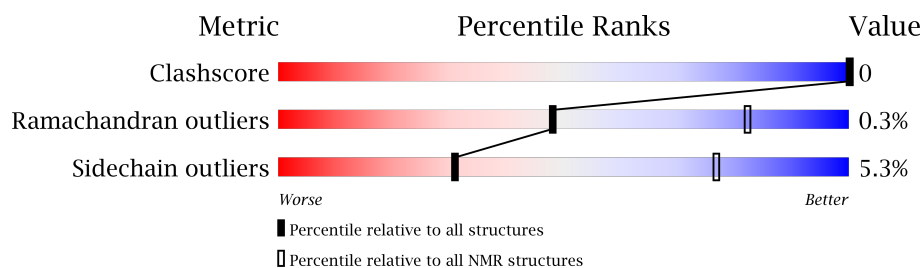
1 Overall quality at a glance

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 ≥ 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	47	 77% . 19%

2 Ensemble composition and analysis

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:30-A:67 (38)	0.09	10

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 8 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 680 atoms, of which 318 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Choline binding protein.

Mol	Chain	Residues	Atoms						Trace
1	A	47	Total	C	H	N	O	S	0
			679	218	318	63	78	2	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	expression tag	UNP A0A0U0AG78
A	25	ALA	-	expression tag	UNP A0A0U0AG78
A	26	SER	-	expression tag	UNP A0A0U0AG78

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

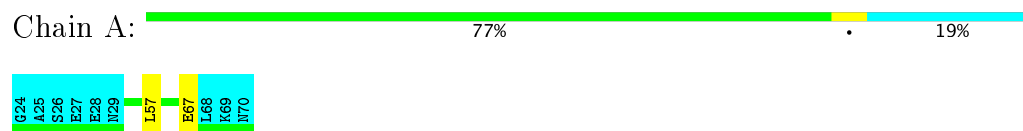
Mol	Chain	Residues	Atoms	
2	A	1	Total	Ca
			1	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

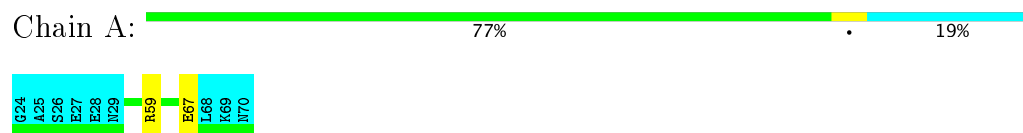
These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain 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: Choline binding protein



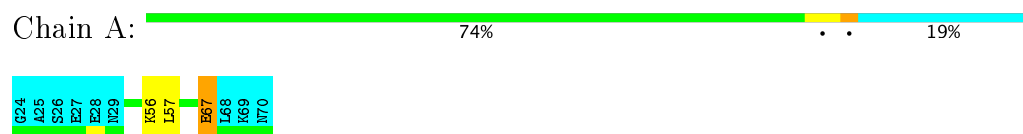
4.2.3 Score per residue for model 3

- Molecule 1: Choline binding protein



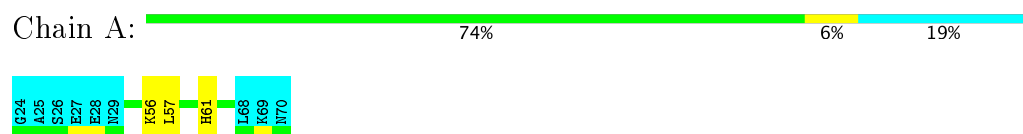
4.2.4 Score per residue for model 4

- Molecule 1: Choline binding protein



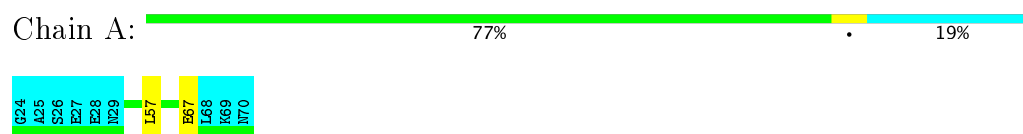
4.2.5 Score per residue for model 5

- Molecule 1: Choline binding protein



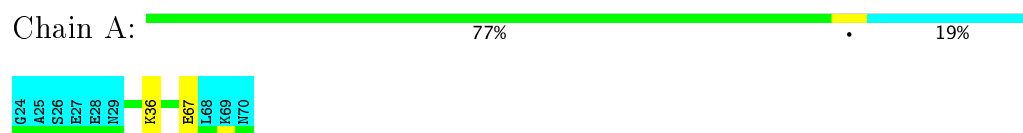
4.2.6 Score per residue for model 6

- Molecule 1: Choline binding protein



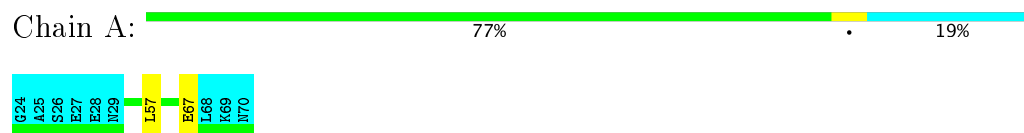
4.2.7 Score per residue for model 7

- Molecule 1: Choline binding protein



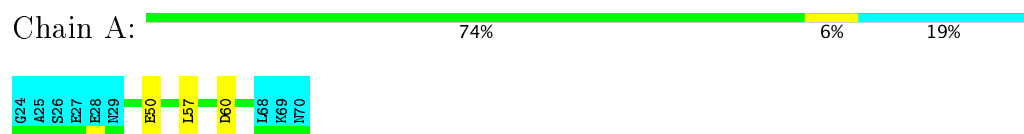
4.2.8 Score per residue for model 8

- Molecule 1: Choline binding protein



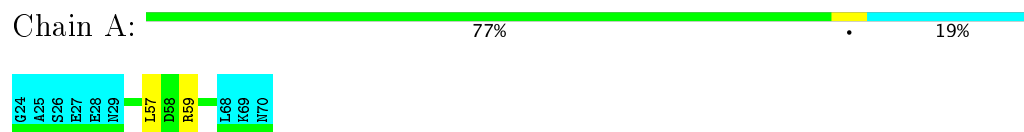
4.2.9 Score per residue for model 9

- Molecule 1: Choline binding protein



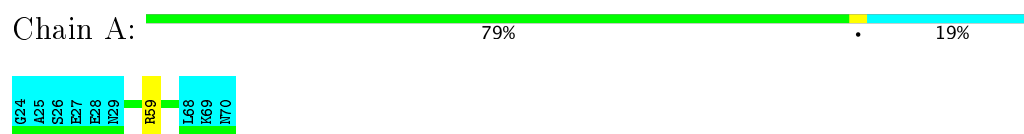
4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Choline binding protein



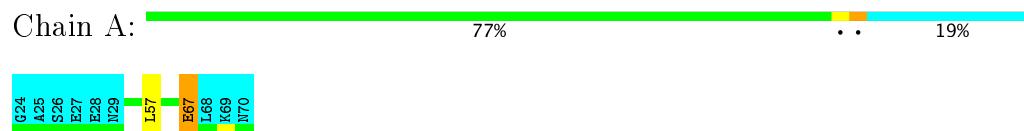
4.2.11 Score per residue for model 11

- Molecule 1: Choline binding protein



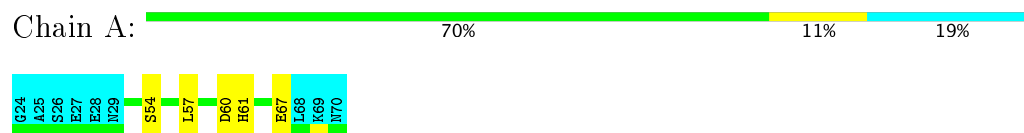
4.2.12 Score per residue for model 12

- Molecule 1: Choline binding protein



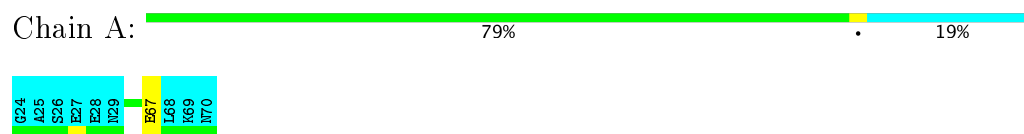
4.2.13 Score per residue for model 13

- Molecule 1: Choline binding protein



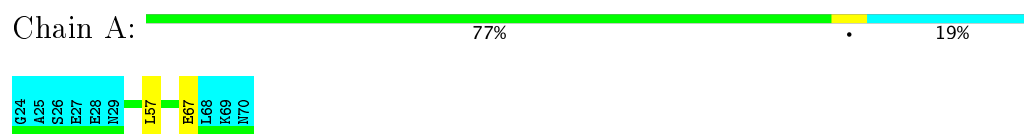
4.2.14 Score per residue for model 14

- Molecule 1: Choline binding protein



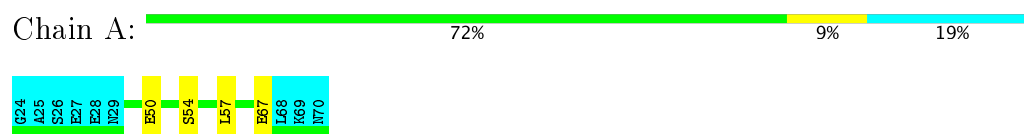
4.2.15 Score per residue for model 15

- Molecule 1: Choline binding protein



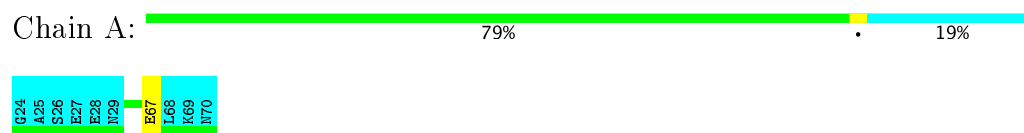
4.2.16 Score per residue for model 16

- Molecule 1: Choline binding protein



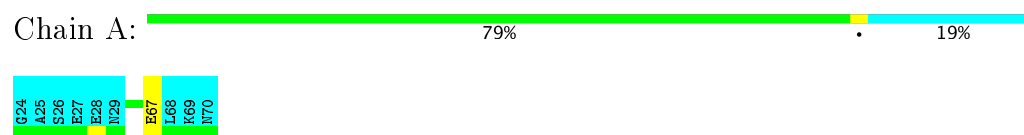
4.2.17 Score per residue for model 17

- Molecule 1: Choline binding protein



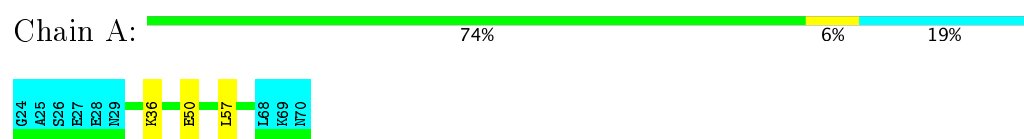
4.2.18 Score per residue for model 18

- Molecule 1: Choline binding protein



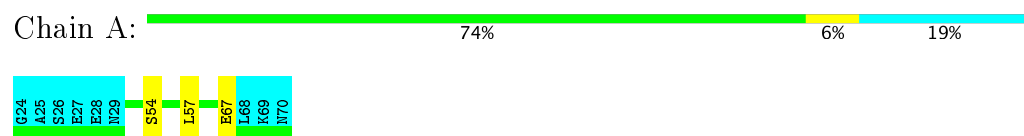
4.2.19 Score per residue for model 19

- Molecule 1: Choline binding protein



4.2.20 Score per residue for model 20

- Molecule 1: Choline binding protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
AMBER	refinement	9.0

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)	5j8t_cs.cif
Number of chemical shift lists	1
Total number of shifts	501
Number of shifts mapped to atoms	0
Number of unparsed shifts	501
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 [i](#)

6.1 Standard geometry [i](#)

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

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	0.76±0.01	0±0/303 (0.0±0.0%)	1.10±0.02	1±1/410 (0.2±0.1%)
All	All	0.76	0/6060 (0.0%)	1.10	16/8200 (0.2%)

There are no bond-length outliers.

All unique angle 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(°)	Ideal(°)	Models	
								Worst	Total
1	A	67	GLU	OE1-CD-OE2	-7.55	114.24	123.30	4	14
1	A	60	ASP	CB-CG-OD2	5.56	123.31	118.30	13	2

There are no chirality outliers.

There are no planarity outliers.

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
All	All	5900	5100	5040	-

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 -.

There are no clashes.

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	38/47 (81%)	37±0 (96±1%)	1±1 (3±1%)	0±0 (0±1%)	48	82
All	All	760/940 (81%)	732 (96%)	26 (3%)	2 (0%)	48	82

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	61	HIS	2

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	30/37 (81%)	28±1 (95±3%)	2±1 (5±3%)	31	77
All	All	600/740 (81%)	568 (95%)	32 (5%)	31	77

All 7 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	57	LEU	14
1	A	59	ARG	4
1	A	50	GLU	4
1	A	54	SER	3
1	A	67	GLU	3
1	A	36	LYS	2
1	A	56	LYS	2

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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: 5j8t_cs.cif

Chemical shift list name: *deposit1num.bmrB*

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	501
Number of shifts mapped to atoms	0
Number of unparsed shifts	501
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 501 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	24	GLY	CA	43.289	0.059	1
2	?	24	GLY	HA2	3.232	0.037	2
3	?	24	GLY	HA3	3.871	0.025	2
4	?	25	ALA	C	178.025	0.000	1
5	?	25	ALA	CA	52.861	0.084	1
6	?	25	ALA	CB	19.197	0.056	1
7	?	25	ALA	HA	4.339	0.036	1
8	?	25	ALA	H	8.600	0.009	1
9	?	25	ALA	N	124.286	0.066	1
10	?	25	ALA	HB1	1.372	0.029	2
11	?	25	ALA	HB2	1.372	0.029	2
12	?	25	ALA	HB3	1.372	0.029	2
13	?	26	SER	C	174.832	0.000	1
14	?	26	SER	CA	58.709	0.093	1
15	?	26	SER	CB	63.693	0.110	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
16	?	26	SER	HA	4.374	0.031	1
17	?	26	SER	HB2	3.811	0.008	2
18	?	26	SER	HB3	3.852	0.006	2
19	?	26	SER	H	8.416	0.020	1
20	?	26	SER	N	115.189	0.054	1
21	?	27	GLU	C	176.393	0.000	1
22	?	27	GLU	CA	56.749	0.096	1
23	?	27	GLU	CB	29.675	0.093	1
24	?	27	GLU	CG	35.425	0.090	1
25	?	27	GLU	HA	4.277	0.034	1
26	?	27	GLU	HB2	1.934	0.039	2
27	?	27	GLU	HB3	2.055	0.027	2
28	?	27	GLU	H	8.366	0.012	1
29	?	27	GLU	N	122.385	0.038	1
30	?	27	GLU	HG2	2.304	0.021	2
31	?	27	GLU	HG3	2.304	0.021	2
32	?	28	GLU	C	175.994	0.000	1
33	?	28	GLU	CA	56.694	0.107	1
34	?	28	GLU	CB	29.800	0.076	1
35	?	28	GLU	CG	35.246	0.106	1
36	?	28	GLU	HA	4.217	0.037	1
37	?	28	GLU	HB2	1.888	0.033	2
38	?	28	GLU	HB3	2.008	0.030	2
39	?	28	GLU	H	8.206	0.012	1
40	?	28	GLU	N	120.797	0.009	1
41	?	28	GLU	HG2	2.275	0.020	2
42	?	28	GLU	HG3	2.275	0.020	2
43	?	29	ASN	C	174.304	0.000	1
44	?	29	ASN	CA	52.974	0.036	1
45	?	29	ASN	CB	38.698	0.177	1
46	?	29	ASN	HA	4.621	0.042	1
47	?	29	ASN	HB2	2.625	0.036	2
48	?	29	ASN	HB3	2.733	0.045	2
49	?	29	ASN	HD21	6.831	0.006	2
50	?	29	ASN	HD22	7.499	0.004	2
51	?	29	ASN	H	8.263	0.006	1
52	?	29	ASN	N	119.797	0.010	1
53	?	29	ASN	ND2	113.001	0.002	1
54	?	30	ILE	C	173.952	0.000	1
55	?	30	ILE	CA	60.502	0.077	1
56	?	30	ILE	CB	38.426	0.113	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
57	?	30	ILE	CD1	12.427	0.046	1
58	?	30	ILE	CG1	26.987	0.030	1
59	?	30	ILE	CG2	16.938	0.075	1
60	?	30	ILE	HA	3.756	0.036	1
61	?	30	ILE	HB	1.365	0.037	1
62	?	30	ILE	HG12	0.753	0.037	1
63	?	30	ILE	HG13	1.077	0.041	2
64	?	30	ILE	H	7.650	0.010	2
65	?	30	ILE	N	121.488	0.034	1
66	?	30	ILE	HD11	0.602	0.036	2
67	?	30	ILE	HD12	0.602	0.036	2
68	?	30	ILE	HD13	0.602	0.036	2
69	?	30	ILE	HG21	0.184	0.035	2
70	?	30	ILE	HG22	0.184	0.035	2
71	?	30	ILE	HG23	0.184	0.035	2
72	?	31	HIS	C	172.297	0.000	1
73	?	31	HIS	CA	54.005	0.108	1
74	?	31	HIS	CB	30.066	0.079	1
75	?	31	HIS	HA	4.383	0.037	1
76	?	31	HIS	HB2	2.827	0.034	2
77	?	31	HIS	HB3	2.920	0.040	2
78	?	31	HIS	HD2	7.031	0.003	1
79	?	31	HIS	HE1	8.445	0.002	1
80	?	31	HIS	H	7.679	0.005	1
81	?	31	HIS	N	122.042	0.017	1
82	?	32	PHE	C	175.501	0.000	1
83	?	32	PHE	CA	55.693	0.139	1
84	?	32	PHE	CB	41.476	0.267	1
85	?	32	PHE	HA	4.924	0.038	1
86	?	32	PHE	HB2	2.366	0.031	2
87	?	32	PHE	HB3	3.126	0.035	2
88	?	32	PHE	H	8.330	0.009	1
89	?	32	PHE	HZ	6.237	0.004	1
90	?	32	PHE	N	121.506	0.019	1
91	?	32	PHE	HD1	6.859	0.004	2
92	?	32	PHE	HD2	6.859	0.004	2
93	?	32	PHE	HE1	6.628	0.003	2
94	?	32	PHE	HE2	6.628	0.003	2
95	?	33	SER	C	173.671	0.000	1
96	?	33	SER	CA	59.356	0.078	1
97	?	33	SER	CB	63.851	0.043	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
98	?	33	SER	HA	4.299	0.037	1
99	?	33	SER	H	9.300	0.031	1
100	?	33	SER	N	117.039	0.031	1
101	?	33	SER	HB2	3.912	0.026	2
102	?	33	SER	HB3	3.912	0.026	2
103	?	34	SER	C	174.316	0.000	1
104	?	34	SER	CA	56.813	0.040	1
105	?	34	SER	CB	65.893	0.237	1
106	?	34	SER	HA	4.458	0.042	1
107	?	34	SER	HB2	3.893	0.029	2
108	?	34	SER	HB3	4.027	0.021	2
109	?	34	SER	H	7.460	0.009	1
110	?	34	SER	N	111.899	0.077	1
111	?	35	CYS	C	174.997	0.000	1
112	?	35	CYS	CA	55.452	0.096	1
113	?	35	CYS	CB	33.316	0.071	1
114	?	35	CYS	HA	4.205	0.049	1
115	?	35	CYS	HB2	1.066	0.026	2
116	?	35	CYS	HB3	2.122	0.035	2
117	?	35	CYS	H	9.214	0.008	1
118	?	35	CYS	N	120.136	0.149	1
119	?	36	LYS	C	179.222	0.000	1
120	?	36	LYS	CA	60.221	0.123	1
121	?	36	LYS	CB	31.942	0.064	1
122	?	36	LYS	CD	29.122	0.129	1
123	?	36	LYS	CE	41.991	0.049	1
124	?	36	LYS	CG	25.015	0.073	1
125	?	36	LYS	HA	3.975	0.037	1
126	?	36	LYS	HG2	1.440	0.027	2
127	?	36	LYS	HG3	1.558	0.041	2
128	?	36	LYS	H	7.893	0.006	1
129	?	36	LYS	N	120.690	0.071	1
130	?	36	LYS	HB2	1.771	0.033	2
131	?	36	LYS	HB3	1.771	0.033	2
132	?	36	LYS	HD2	1.702	0.032	2
133	?	36	LYS	HD3	1.702	0.032	2
134	?	36	LYS	HE2	3.000	0.038	2
135	?	36	LYS	HE3	3.000	0.038	2
136	?	37	GLU	C	178.142	0.000	1
137	?	37	GLU	CA	58.824	0.118	1
138	?	37	GLU	CB	30.211	0.153	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
139	?	37	GLU	CG	36.263	0.087	1
140	?	37	GLU	HA	4.030	0.034	1
141	?	37	GLU	HB2	2.046	0.030	2
142	?	37	GLU	HB3	2.192	0.033	2
143	?	37	GLU	HG2	2.263	0.031	2
144	?	37	GLU	HG3	2.376	0.028	2
145	?	37	GLU	H	7.397	0.006	1
146	?	37	GLU	N	119.946	0.002	1
147	?	38	ALA	C	180.184	0.000	1
148	?	38	ALA	CA	55.656	0.057	1
149	?	38	ALA	CB	17.537	0.085	1
150	?	38	ALA	HA	2.409	0.032	1
151	?	38	ALA	H	7.050	0.005	1
152	?	38	ALA	N	123.887	0.050	1
153	?	38	ALA	HB1	0.720	0.035	2
154	?	38	ALA	HB2	0.720	0.035	2
155	?	38	ALA	HB3	0.720	0.035	2
156	?	39	TRP	C	181.428	0.000	1
157	?	39	TRP	CA	58.288	0.135	1
158	?	39	TRP	CB	28.353	0.050	1
159	?	39	TRP	HA	4.712	0.039	1
160	?	39	TRP	HB2	3.112	0.030	2
161	?	39	TRP	HB3	3.283	0.033	2
162	?	39	TRP	HD1	7.740	0.002	1
163	?	39	TRP	HE1	9.478	0.003	2
164	?	39	TRP	HE3	7.411	0.003	2
165	?	39	TRP	HH2	7.120	0.006	1
166	?	39	TRP	H	8.833	0.007	1
167	?	39	TRP	HZ2	7.192	0.008	2
168	?	39	TRP	HZ3	6.986	0.002	2
169	?	39	TRP	N	119.842	0.017	1
170	?	39	TRP	NE1	126.423	0.000	1
171	?	40	ALA	C	178.541	0.000	1
172	?	40	ALA	CA	54.616	0.068	1
173	?	40	ALA	CB	18.031	0.048	1
174	?	40	ALA	HA	4.220	0.036	1
175	?	40	ALA	H	8.012	0.011	1
176	?	40	ALA	N	122.387	0.047	1
177	?	40	ALA	HB1	1.557	0.037	2
178	?	40	ALA	HB2	1.557	0.037	2
179	?	40	ALA	HB3	1.557	0.037	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
180	?	41	ASN	C	174.316	0.000	1
181	?	41	ASN	CA	53.740	0.152	1
182	?	41	ASN	CB	41.003	0.136	1
183	?	41	ASN	HA	4.852	0.040	1
184	?	41	ASN	HB2	2.738	0.036	2
185	?	41	ASN	HB3	3.229	0.036	2
186	?	41	ASN	HD21	7.394	0.008	2
187	?	41	ASN	HD22	7.756	0.005	2
188	?	41	ASN	H	7.579	0.010	1
189	?	41	ASN	N	115.100	0.001	1
190	?	41	ASN	ND2	115.928	0.002	1
191	?	42	GLY	C	174.046	0.000	1
192	?	42	GLY	CA	46.002	0.048	1
193	?	42	GLY	HA2	3.714	0.038	2
194	?	42	GLY	HA3	4.080	0.039	2
195	?	42	GLY	H	7.913	0.010	1
196	?	42	GLY	N	107.010	0.083	1
197	?	43	TYR	C	173.706	0.000	1
198	?	43	TYR	CA	57.379	0.075	1
199	?	43	TYR	CB	40.152	0.036	1
200	?	43	TYR	HA	4.677	0.022	1
201	?	43	TYR	H	8.349	0.008	1
202	?	43	TYR	N	122.311	0.078	1
203	?	43	TYR	HB2	2.506	0.029	2
204	?	43	TYR	HB3	2.506	0.029	2
205	?	43	TYR	HD1	7.024	0.002	2
206	?	43	TYR	HD2	7.024	0.002	2
207	?	43	TYR	HE1	6.834	0.002	2
208	?	43	TYR	HE2	6.834	0.002	2
209	?	44	SER	C	171.992	0.000	1
210	?	44	SER	CA	57.739	0.053	1
211	?	44	SER	CB	65.629	0.040	1
212	?	44	SER	HA	4.470	0.038	1
213	?	44	SER	H	7.942	0.006	1
214	?	44	SER	N	110.543	0.014	1
215	?	44	SER	HB2	3.995	0.037	2
216	?	44	SER	HB3	3.995	0.037	2
217	?	45	ASP	C	174.680	0.000	1
218	?	45	ASP	CA	55.742	0.033	1
219	?	45	ASP	CB	39.194	0.090	1
220	?	45	ASP	HA	3.709	0.034	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
221	?	45	ASP	HB2	2.654	0.012	2
222	?	45	ASP	HB3	2.781	0.024	2
223	?	45	ASP	H	8.127	0.014	1
224	?	45	ASP	N	119.298	0.006	1
225	?	46	ILE	C	177.097	0.000	1
226	?	46	ILE	CA	61.981	0.070	1
227	?	46	ILE	CB	40.542	0.079	1
228	?	46	ILE	CD1	14.154	0.070	1
229	?	46	ILE	CG1	26.732	0.062	1
230	?	46	ILE	CG2	18.614	0.128	1
231	?	46	ILE	HA	3.993	0.039	1
232	?	46	ILE	HB	1.670	0.036	1
233	?	46	ILE	HG12	1.090	0.036	2
234	?	46	ILE	HG13	1.358	0.034	2
235	?	46	ILE	H	8.377	0.008	1
236	?	46	ILE	N	118.575	0.044	1
237	?	46	ILE	HD11	0.650	0.035	2
238	?	46	ILE	HD12	0.650	0.035	2
239	?	46	ILE	HD13	0.650	0.035	2
240	?	46	ILE	HG21	0.995	0.039	2
241	?	46	ILE	HG22	0.995	0.039	2
242	?	46	ILE	HG23	0.995	0.039	2
243	?	47	HIS	C	174.375	0.000	1
244	?	47	HIS	CA	56.218	0.049	1
245	?	47	HIS	CB	29.067	0.075	1
246	?	47	HIS	HA	4.942	0.042	1
247	?	47	HIS	HB2	2.977	0.037	2
248	?	47	HIS	HB3	3.264	0.037	2
249	?	47	HIS	HD2	7.477	0.001	1
250	?	47	HIS	HE1	8.602	0.003	1
251	?	47	HIS	H	9.383	0.035	1
252	?	47	HIS	N	128.636	0.030	1
253	?	48	GLU	C	176.487	0.000	1
254	?	48	GLU	CA	58.066	0.100	1
255	?	48	GLU	CB	28.428	0.090	1
256	?	48	GLU	CG	34.504	0.084	1
257	?	48	GLU	HA	2.496	0.033	1
258	?	48	GLU	HB2	1.144	0.036	2
259	?	48	GLU	HB3	1.534	0.031	2
260	?	48	GLU	H	7.787	0.005	1
261	?	48	GLU	N	122.093	0.016	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
262	?	48	GLU	HG2	1.895	0.024	2
263	?	48	GLU	HG3	1.895	0.024	2
264	?	49	GLY	C	174.293	0.000	1
265	?	49	GLY	CA	44.997	0.035	1
266	?	49	GLY	HA2	3.605	0.038	2
267	?	49	GLY	HA3	4.245	0.039	2
268	?	49	GLY	H	8.145	0.007	1
269	?	49	GLY	N	114.595	0.016	1
270	?	50	GLU	CA	53.930	0.101	1
271	?	50	GLU	CB	28.395	0.106	1
272	?	50	GLU	CG	36.402	0.009	1
273	?	50	GLU	HA	4.781	0.032	1
274	?	50	GLU	HB2	2.209	0.028	2
275	?	50	GLU	HB3	2.465	0.041	2
276	?	50	GLU	HG2	2.375	0.026	2
277	?	50	GLU	HG3	2.324	0.064	2
278	?	50	GLU	H	8.154	0.020	1
279	?	50	GLU	N	120.694	0.023	1
280	?	51	PRO	C	176.170	0.000	1
281	?	51	PRO	CA	64.191	0.120	1
282	?	51	PRO	CB	32.043	0.035	1
283	?	51	PRO	CD	50.769	0.067	1
284	?	51	PRO	CG	27.892	0.029	1
285	?	51	PRO	HA	4.283	0.035	1
286	?	51	PRO	HB2	1.947	0.059	2
287	?	51	PRO	HB3	2.355	0.032	2
288	?	51	PRO	HD2	3.958	0.049	2
289	?	51	PRO	HD3	3.786	0.037	2
290	?	51	PRO	HG2	2.046	0.034	2
291	?	51	PRO	HG3	2.243	0.040	2
292	?	52	GLY	C	174.692	0.000	1
293	?	52	GLY	CA	44.786	0.133	1
294	?	52	GLY	HA2	3.217	0.038	2
295	?	52	GLY	HA3	4.077	0.038	2
296	?	52	GLY	H	8.484	0.010	1
297	?	52	GLY	N	109.195	0.054	1
298	?	53	TYR	CA	62.172	0.123	1
299	?	53	TYR	CB	37.987	0.032	1
300	?	53	TYR	HA	3.438	0.038	1
301	?	53	TYR	HB2	2.940	0.035	2
302	?	53	TYR	HB3	3.009	0.046	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
303	?	53	TYR	H	7.680	0.012	1
304	?	53	TYR	N	120.719	0.078	1
305	?	53	TYR	HD1	6.942	0.002	2
306	?	53	TYR	HD2	6.942	0.002	2
307	?	54	SER	C	174.140	0.000	1
308	?	54	SER	CA	56.419	0.044	1
309	?	54	SER	CB	65.311	0.027	1
310	?	54	SER	HA	4.300	0.012	1
311	?	54	SER	HB2	3.347	0.004	2
312	?	54	SER	HB3	3.838	0.004	2
313	?	54	SER	H	5.349	0.007	1
314	?	54	SER	N	119.057	0.021	1
315	?	55	ALA	C	180.125	0.000	1
316	?	55	ALA	CA	55.025	0.090	1
317	?	55	ALA	CB	18.121	0.160	1
318	?	55	ALA	HA	4.030	0.039	1
319	?	55	ALA	H	9.037	0.011	1
320	?	55	ALA	N	129.807	0.029	1
321	?	55	ALA	HB1	1.529	0.038	2
322	?	55	ALA	HB2	1.529	0.038	2
323	?	55	ALA	HB3	1.529	0.038	2
324	?	56	LYS	C	177.403	0.000	1
325	?	56	LYS	CA	58.189	0.030	1
326	?	56	LYS	CB	32.146	0.075	1
327	?	56	LYS	CD	29.032	0.077	1
328	?	56	LYS	CE	42.197	0.098	1
329	?	56	LYS	CG	24.808	0.080	1
330	?	56	LYS	HA	3.996	0.035	1
331	?	56	LYS	H	7.841	0.012	1
332	?	56	LYS	N	115.889	0.046	1
333	?	56	LYS	HB2	1.709	0.033	2
334	?	56	LYS	HB3	1.709	0.033	2
335	?	56	LYS	HD2	1.615	0.032	2
336	?	56	LYS	HD3	1.615	0.032	2
337	?	56	LYS	HE2	2.956	0.032	2
338	?	56	LYS	HE3	2.956	0.032	2
339	?	56	LYS	HG2	1.362	0.042	2
340	?	56	LYS	HG3	1.362	0.042	2
341	?	57	LEU	C	175.619	0.000	1
342	?	57	LEU	CA	54.384	0.078	1
343	?	57	LEU	CB	41.347	0.068	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
344	?	57	LEU	CD1	25.239	0.106	1
345	?	57	LEU	CD2	21.308	0.066	1
346	?	57	LEU	CG	26.454	0.083	1
347	?	57	LEU	HA	4.208	0.042	1
348	?	57	LEU	HB2	1.348	0.029	2
349	?	57	LEU	HB3	1.749	0.042	2
350	?	57	LEU	HG	1.336	0.051	1
351	?	57	LEU	H	6.918	0.007	1
352	?	57	LEU	N	116.062	0.032	1
353	?	57	LEU	HD11	0.496	0.034	2
354	?	57	LEU	HD12	0.496	0.034	2
355	?	57	LEU	HD13	0.496	0.034	2
356	?	57	LEU	HD21	0.654	0.033	2
357	?	57	LEU	HD22	0.654	0.033	2
358	?	57	LEU	HD23	0.654	0.033	2
359	?	58	ASP	C	176.264	0.000	1
360	?	58	ASP	CA	51.287	0.089	1
361	?	58	ASP	CB	40.197	0.056	1
362	?	58	ASP	HA	5.194	0.060	1
363	?	58	ASP	HB2	2.079	0.035	2
364	?	58	ASP	HB3	3.088	0.041	2
365	?	58	ASP	H	7.187	0.008	1
366	?	58	ASP	N	121.031	0.031	1
367	?	59	ARG	C	176.605	0.000	1
368	?	59	ARG	CA	59.173	0.085	1
369	?	59	ARG	CB	29.988	0.055	1
370	?	59	ARG	CD	43.161	0.088	1
371	?	59	ARG	CG	27.204	0.127	1
372	?	59	ARG	HA	3.898	0.040	1
373	?	59	ARG	HE	7.177	0.003	1
374	?	59	ARG	H	7.878	0.018	1
375	?	59	ARG	N	122.200	0.001	1
376	?	59	ARG	HB2	1.851	0.034	2
377	?	59	ARG	HB3	1.851	0.034	2
378	?	59	ARG	HD2	3.237	0.032	2
379	?	59	ARG	HD3	3.237	0.032	2
380	?	59	ARG	HG2	1.694	0.033	2
381	?	59	ARG	HG3	1.694	0.033	2
382	?	60	ASP	C	175.466	0.000	1
383	?	60	ASP	CA	52.081	0.105	1
384	?	60	ASP	CB	38.880	0.043	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
385	?	60	ASP	HA	4.456	0.035	1
386	?	60	ASP	HB2	2.497	0.031	1
387	?	60	ASP	HB3	2.942	0.037	1
388	?	60	ASP	H	7.997	0.004	1
389	?	60	ASP	N	113.599	0.003	1
390	?	61	HIS	C	174.152	0.000	1
391	?	61	HIS	CA	55.947	0.071	1
392	?	61	HIS	CB	26.400	0.073	1
393	?	61	HIS	HA	4.253	0.035	1
394	?	61	HIS	HB2	3.322	0.032	2
395	?	61	HIS	HB3	3.382	0.038	2
396	?	61	HIS	HD2	7.198	0.002	1
397	?	61	HIS	HE1	8.498	0.002	1
398	?	61	HIS	H	7.563	0.003	1
399	?	61	HIS	N	115.599	0.003	1
400	?	62	ASP	C	177.356	0.000	1
401	?	62	ASP	CA	52.986	0.026	1
402	?	62	ASP	CB	40.903	0.043	1
403	?	62	ASP	HA	4.714	0.006	1
404	?	62	ASP	HB2	2.390	0.009	2
405	?	62	ASP	HB3	3.029	0.003	2
406	?	62	ASP	H	8.398	0.005	1
407	?	62	ASP	N	117.996	0.014	1
408	?	63	GLY	C	173.225	0.000	1
409	?	63	GLY	CA	45.319	0.139	1
410	?	63	GLY	HA2	3.429	0.036	2
411	?	63	GLY	HA3	4.234	0.037	2
412	?	63	GLY	H	9.781	0.007	1
413	?	63	GLY	N	111.703	0.055	1
414	?	64	VAL	C	174.727	0.000	1
415	?	64	VAL	CA	60.952	0.090	1
416	?	64	VAL	CB	33.100	0.131	1
417	?	64	VAL	CG1	20.380	0.138	1
418	?	64	VAL	CG2	21.585	0.072	1
419	?	64	VAL	HA	4.568	0.042	1
420	?	64	VAL	HB	1.870	0.036	1
421	?	64	VAL	H	7.770	0.006	1
422	?	64	VAL	N	120.691	0.028	1
423	?	64	VAL	HG11	0.384	0.033	2
424	?	64	VAL	HG12	0.384	0.033	2
425	?	64	VAL	HG13	0.384	0.033	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
426	?	64	VAL	HG21	0.504	0.033	2
427	?	64	VAL	HG22	0.504	0.033	2
428	?	64	VAL	HG23	0.504	0.033	2
429	?	65	ALA	C	176.440	0.000	1
430	?	65	ALA	CA	50.455	0.059	1
431	?	65	ALA	CB	21.616	0.034	1
432	?	65	ALA	HA	4.739	0.039	1
433	?	65	ALA	H	10.303	0.028	1
434	?	65	ALA	N	131.863	0.070	1
435	?	65	ALA	HB1	1.252	0.035	2
436	?	65	ALA	HB2	1.252	0.035	2
437	?	65	ALA	HB3	1.252	0.035	2
438	?	66	CYS	C	176.875	0.000	1
439	?	66	CYS	CA	53.021	0.076	1
440	?	66	CYS	CB	31.308	0.019	1
441	?	66	CYS	HA	4.737	0.034	1
442	?	66	CYS	HB2	2.672	0.026	2
443	?	66	CYS	HB3	2.983	0.024	2
444	?	66	CYS	H	8.587	0.013	1
445	?	66	CYS	N	115.105	0.044	1
446	?	67	GLU	C	176.851	0.000	1
447	?	67	GLU	CA	57.511	0.045	1
448	?	67	GLU	CB	29.621	0.022	1
449	?	67	GLU	CG	36.423	0.037	1
450	?	67	GLU	HA	4.409	0.032	1
451	?	67	GLU	HB2	2.207	0.001	2
452	?	67	GLU	HB3	2.005	0.005	2
453	?	67	GLU	HG2	2.311	0.005	2
454	?	67	GLU	HG3	2.425	0.001	2
455	?	67	GLU	H	9.568	0.006	1
456	?	67	GLU	N	124.654	0.051	1
457	?	68	LEU	C	177.097	0.000	1
458	?	68	LEU	CA	55.542	0.097	1
459	?	68	LEU	CB	42.955	0.090	1
460	?	68	LEU	CD1	23.160	0.057	1
461	?	68	LEU	CD2	24.008	0.067	1
462	?	68	LEU	CG	26.736	0.097	1
463	?	68	LEU	HA	4.137	0.036	1
464	?	68	LEU	HB2	1.381	0.042	2
465	?	68	LEU	HB3	1.468	0.044	2
466	?	68	LEU	HG	1.322	0.038	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
467	?	68	LEU	H	8.748	0.050	1
468	?	68	LEU	N	124.460	0.023	1
469	?	68	LEU	HD11	0.201	0.035	2
470	?	68	LEU	HD12	0.201	0.035	2
471	?	68	LEU	HD13	0.201	0.035	2
472	?	68	LEU	HD21	0.438	0.034	2
473	?	68	LEU	HD22	0.438	0.034	2
474	?	68	LEU	HD23	0.438	0.034	2
475	?	69	LYS	C	175.161	0.000	1
476	?	69	LYS	CA	55.991	0.051	1
477	?	69	LYS	CB	33.008	0.053	1
478	?	69	LYS	CD	28.985	0.068	1
479	?	69	LYS	CE	42.021	0.038	1
480	?	69	LYS	CG	24.366	0.075	1
481	?	69	LYS	HA	4.285	0.036	1
482	?	69	LYS	HB2	1.679	0.000	2
483	?	69	LYS	HB3	1.815	0.024	2
484	?	69	LYS	H	8.260	0.023	1
485	?	69	LYS	N	122.600	0.002	1
486	?	69	LYS	HD2	1.626	0.035	2
487	?	69	LYS	HD3	1.626	0.035	2
488	?	69	LYS	HE2	2.934	0.042	2
489	?	69	LYS	HE3	2.934	0.042	2
490	?	69	LYS	HG2	1.313	0.029	2
491	?	69	LYS	HG3	1.313	0.029	2
492	?	70	ASN	CA	54.629	0.104	1
493	?	70	ASN	CB	40.240	0.061	1
494	?	70	ASN	HA	4.400	0.041	1
495	?	70	ASN	HB2	2.586	0.030	2
496	?	70	ASN	HB3	2.685	0.033	2
497	?	70	ASN	HD21	6.729	0.005	2
498	?	70	ASN	HD22	7.436	0.007	2
499	?	70	ASN	H	7.967	0.007	1
500	?	70	ASN	N	125.702	0.008	1
501	?	70	ASN	ND2	113.336	0.034	1

7.1.2 Chemical shift referencing ⓘ

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

7.1.3 Completeness of resonance assignments [i](#)

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 433. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/188 (0%)	0/75 (0%)	0/76 (0%)	0/37 (0%)
Sidechain	0/184 (0%)	0/109 (0%)	0/69 (0%)	0/6 (0%)
Aromatic	0/61 (0%)	0/31 (0%)	0/23 (0%)	0/7 (0%)
Overall	0/433 (0%)	0/215 (0%)	0/168 (0%)	0/50 (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 533. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/233 (0%)	0/93 (0%)	0/94 (0%)	0/46 (0%)
Sidechain	0/239 (0%)	0/141 (0%)	0/89 (0%)	0/9 (0%)
Aromatic	0/61 (0%)	0/31 (0%)	0/23 (0%)	0/7 (0%)
Overall	0/533 (0%)	0/265 (0%)	0/206 (0%)	0/62 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (deposit1num.bmr). RCI is only applicable to proteins.