



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 6D10
BMRB ID : 30450
Title : CS-rosetta determined structures of the C-terminal domain of AlgF from *P. aeruginosa*
Authors : Tammam, S.; Howell, P.L.
Deposited on : 2018-04-11

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

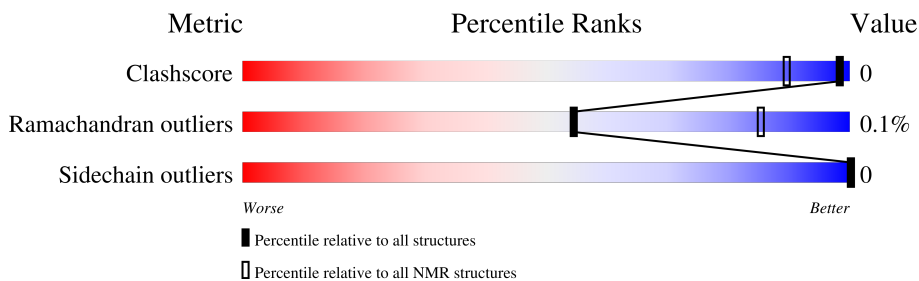
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR, SOLUTION SCATTERING

The overall completeness of chemical shifts assignment is 93%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	196	

2 Ensemble composition and analysis

This entry contains 10 models. Model 5 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:126-A:212 (87)	1.85	5

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 2 clusters and 4 single-model clusters were found.

Cluster number	Models
1	4, 5, 6, 10
2	7, 8
Single-model clusters	1; 2; 3; 9

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1386 atoms, of which 718 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Alginate biosynthesis protein AlgF.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	89	1386	422	718	122	123	1	0

There are 9 discrepancies between the modelled and reference sequences:

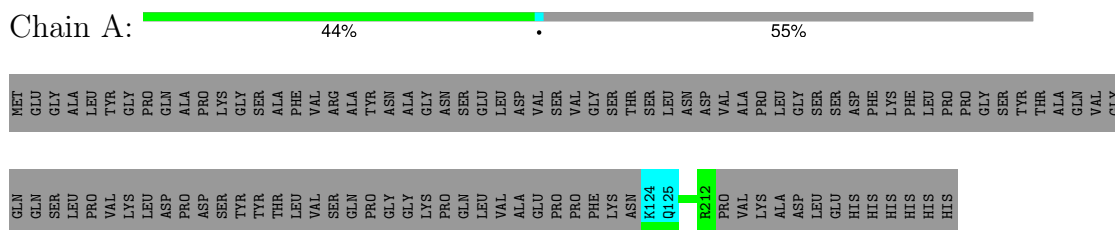
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	initiating methionine	UNP Q06062
A	218	LEU	-	expression tag	UNP Q06062
A	219	GLU	-	expression tag	UNP Q06062
A	220	HIS	-	expression tag	UNP Q06062
A	221	HIS	-	expression tag	UNP Q06062
A	222	HIS	-	expression tag	UNP Q06062
A	223	HIS	-	expression tag	UNP Q06062
A	224	HIS	-	expression tag	UNP Q06062
A	225	HIS	-	expression tag	UNP Q06062

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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.

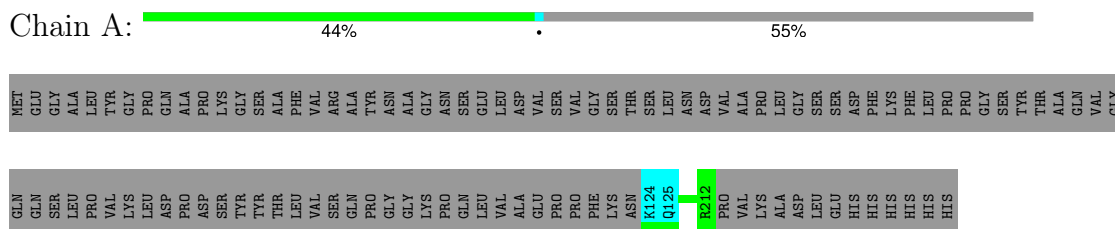
- Molecule 1: Alginate biosynthesis protein AlgF



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 5. Colouring as in section 4.1 above.

- Molecule 1: Alginate biosynthesis protein AlgF



5 Refinement protocol and experimental data overview

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

Of the 3000 calculated structures, 10 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
CS-ROSETTA	refinement	
CS-ROSETTA	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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2322
Number of shifts mapped to atoms	1124
Number of unparsed shifts	0
Number of shifts with mapping errors	1198
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 [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	650	697	697	0±0
All	All	6500	6970	6970	3

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:ARG:HH21	1:A:159:HIS:CE1	0.47	2.27	7	1
1:A:183:LEU:O	1:A:184:LYS:HB2	0.47	2.09	1	1
1:A:209:TRP:CD1	1:A:209:TRP:C	0.43	2.89	8	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	86/196 (44%)	82±2 (95±2%)	4±2 (4±2%)	0±0 (0±0%)	54	85
All	All	860/1960 (44%)	821 (95%)	38 (4%)	1 (0%)	54	85

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	160	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	73/163 (45%)	73±0 (100±0%)	0±0 (0±0%)	100	100
All	All	730/1630 (45%)	730 (100%)	0 (0%)	100	100

There are no protein residues with a non-rotameric sidechain to report.

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 monosaccharides 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 i

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 93% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *NMRstarSubmit.str*

7.1.1 Bookkeeping i

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	2322
Number of shifts mapped to atoms	1124
Number of unparsed shifts	0
Number of shifts with mapping errors	1198
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 1198) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	30	MET	CA	53.231	0.000	.
1	A	30	MET	HA	4.827	0.000	.
1	A	30	MET	C	172.77	0.000	.
1	A	31	GLU	N	120.927	0.000	.
1	A	31	GLU	H	8.209	0.000	.
1	A	31	GLU	CA	56.546	0.017	.
1	A	31	GLU	HA	4.318	0.005	.
1	A	31	GLU	CB	30.381	0.021	.
1	A	31	GLU	HB2	2.037	0.005	.
1	A	31	GLU	HB3	1.939	0.007	.
1	A	31	GLU	CG	36.276	0.054	.
1	A	31	GLU	HG2	2.249	0.002	.
1	A	31	GLU	HG3	2.249	0.002	.
1	A	31	GLU	C	176.656	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	32	GLY	N	110.568	0.012	.
1	A	32	GLY	H	8.541	0.004	.
1	A	32	GLY	CA	45.308	0.000	.
1	A	32	GLY	HA2	3.945	0.005	.
1	A	32	GLY	HA3	3.909	0.000	.
1	A	32	GLY	C	173.757	0.000	.
1	A	33	ALA	N	123.441	0.012	.
1	A	33	ALA	H	8.14	0.006	.
1	A	33	ALA	CA	52.481	0.006	.
1	A	33	ALA	HA	4.259	0.013	.
1	A	33	ALA	HB1	1.308	0.009	.
1	A	33	ALA	HB2	1.308	0.009	.
1	A	33	ALA	HB3	1.308	0.009	.
1	A	33	ALA	CB	19.474	0.000	.
1	A	33	ALA	C	177.599	0.000	.
1	A	34	LEU	N	120.893	0.005	.
1	A	34	LEU	H	8.138	0.003	.
1	A	34	LEU	CA	55.275	0.005	.
1	A	34	LEU	HA	4.218	0.006	.
1	A	34	LEU	CB	42.354	0.006	.
1	A	34	LEU	HB2	1.448	0.004	.
1	A	34	LEU	HB3	1.334	0.002	.
1	A	34	LEU	CG	27.334	0.000	.
1	A	34	LEU	HG	1.447	0.014	.
1	A	34	LEU	HD11	0.826	0.006	.
1	A	34	LEU	HD12	0.826	0.006	.
1	A	34	LEU	HD13	0.826	0.006	.
1	A	34	LEU	HD21	0.777	0.004	.
1	A	34	LEU	HD22	0.777	0.004	.
1	A	34	LEU	HD23	0.777	0.004	.
1	A	34	LEU	CD1	24.967	0.043	.
1	A	34	LEU	CD2	23.705	0.058	.
1	A	34	LEU	C	176.888	0.000	.
1	A	35	TYR	N	119.454	0.038	.
1	A	35	TYR	H	8.038	0.002	.
1	A	35	TYR	CA	57.319	0.004	.
1	A	35	TYR	HA	4.629	0.003	.
1	A	35	TYR	CB	39.054	0.010	.
1	A	35	TYR	HB2	3.107	0.004	.
1	A	35	TYR	HB3	2.889	0.006	.
1	A	35	TYR	HD1	7.083	0.001	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	35	TYR	HD2	7.083	0.001	.
1	A	35	TYR	HE1	6.776	0.000	.
1	A	35	TYR	HE2	6.776	0.000	.
1	A	35	TYR	CD1	133.28	0.004	.
1	A	35	TYR	CE1	118.15	0.000	.
1	A	35	TYR	C	175.888	0.000	.
1	A	36	GLY	N	110.044	0.008	.
1	A	36	GLY	H	8.097	0.002	.
1	A	36	GLY	CA	44.622	0.012	.
1	A	36	GLY	HA2	4.067	0.007	.
1	A	36	GLY	HA3	4.067	0.007	.
1	A	36	GLY	C	175.884	0.000	.
1	A	37	PRO	CD	49.881	0.028	.
1	A	37	PRO	CA	63.122	0.057	.
1	A	37	PRO	HA	4.455	0.008	.
1	A	37	PRO	CB	32.316	0.047	.
1	A	37	PRO	HB2	2.356	0.005	.
1	A	37	PRO	HB3	2.002	0.012	.
1	A	37	PRO	CG	27.442	0.011	.
1	A	37	PRO	HG2	2.078	0.005	.
1	A	37	PRO	HG3	2.078	0.005	.
1	A	37	PRO	HD2	3.644	0.011	.
1	A	37	PRO	HD3	3.607	0.010	.
1	A	37	PRO	C	176.828	0.000	.
1	A	38	GLN	N	120.514	0.012	.
1	A	38	GLN	H	8.432	0.002	.
1	A	38	GLN	CA	54.915	0.047	.
1	A	38	GLN	HA	4.263	0.002	.
1	A	38	GLN	CB	29.766	0.013	.
1	A	38	GLN	HB2	1.993	0.007	.
1	A	38	GLN	HB3	1.881	0.002	.
1	A	38	GLN	CG	33.849	0.004	.
1	A	38	GLN	HG2	2.328	0.007	.
1	A	38	GLN	HG3	2.328	0.007	.
1	A	38	GLN	CD	179.86	0.000	.
1	A	38	GLN	NE2	110.55	0.042	.
1	A	38	GLN	HE21	7.794	0.004	.
1	A	38	GLN	HE22	7.014	0.003	.
1	A	38	GLN	C	175.138	0.000	.
1	A	39	ALA	N	127.209	0.040	.
1	A	39	ALA	H	8.201	0.003	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	39	ALA	CA	49.912	0.018	.
1	A	39	ALA	HA	3.174	0.013	.
1	A	39	ALA	HB1	0.835	0.008	.
1	A	39	ALA	HB2	0.835	0.008	.
1	A	39	ALA	HB3	0.835	0.008	.
1	A	39	ALA	CB	19.14	0.039	.
1	A	39	ALA	C	175.138	0.000	.
1	A	40	PRO	CD	51.006	0.041	.
1	A	40	PRO	CA	62.197	0.034	.
1	A	40	PRO	HA	4.259	0.007	.
1	A	40	PRO	CB	32.121	0.050	.
1	A	40	PRO	HB2	1.563	0.012	.
1	A	40	PRO	HB3	2.227	0.007	.
1	A	40	PRO	CG	27.557	0.025	.
1	A	40	PRO	HG2	1.872	0.006	.
1	A	40	PRO	HG3	1.793	0.009	.
1	A	40	PRO	HD2	2.823	0.008	.
1	A	40	PRO	HD3	3.286	0.008	.
1	A	41	LYS	CA	58.005	0.043	.
1	A	41	LYS	HA	4.075	0.004	.
1	A	41	LYS	CB	32.077	0.000	.
1	A	41	LYS	HB2	1.773	0.012	.
1	A	41	LYS	HB3	1.774	0.012	.
1	A	41	LYS	CG	24.831	0.050	.
1	A	41	LYS	HG2	1.523	0.008	.
1	A	41	LYS	HG3	1.43	0.008	.
1	A	41	LYS	CD	28.967	0.017	.
1	A	41	LYS	HD2	1.676	0.004	.
1	A	41	LYS	HD3	1.676	0.004	.
1	A	41	LYS	CE	41.839	0.074	.
1	A	41	LYS	HE2	2.975	0.006	.
1	A	41	LYS	HE3	2.901	0.013	.
1	A	41	LYS	C	177.322	0.000	.
1	A	42	GLY	N	114.99	0.029	.
1	A	42	GLY	H	8.99	0.006	.
1	A	42	GLY	CA	45.224	0.031	.
1	A	42	GLY	HA2	4.159	0.007	.
1	A	42	GLY	HA3	3.699	0.012	.
1	A	42	GLY	C	173.944	0.000	.
1	A	43	SER	N	113.585	0.025	.
1	A	43	SER	H	7.349	0.004	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	43	SER	CA	61.331	0.034	.
1	A	43	SER	HA	4.089	0.009	.
1	A	43	SER	CB	64.406	0.024	.
1	A	43	SER	HB2	3.506	0.008	.
1	A	43	SER	HB3	3.177	0.008	.
1	A	43	SER	C	173.668	0.000	.
1	A	44	ALA	N	124.859	0.017	.
1	A	44	ALA	H	8.669	0.002	.
1	A	44	ALA	CA	50.573	0.015	.
1	A	44	ALA	HA	4.987	0.013	.
1	A	44	ALA	HB1	1.342	0.008	.
1	A	44	ALA	HB2	1.342	0.008	.
1	A	44	ALA	HB3	1.342	0.008	.
1	A	44	ALA	CB	21.841	0.030	.
1	A	44	ALA	C	175.564	0.000	.
1	A	45	PHE	N	115.268	0.027	.
1	A	45	PHE	H	8.584	0.006	.
1	A	45	PHE	CA	56.556	0.019	.
1	A	45	PHE	HA	5.376	0.009	.
1	A	45	PHE	CB	43.704	0.028	.
1	A	45	PHE	HB2	2.307	0.010	.
1	A	45	PHE	HB3	1.943	0.013	.
1	A	45	PHE	HD1	6.304	0.008	.
1	A	45	PHE	HD2	6.304	0.008	.
1	A	45	PHE	HE1	6.987	0.008	.
1	A	45	PHE	HE2	6.987	0.008	.
1	A	45	PHE	CZ	129.04	0.000	.
1	A	45	PHE	HZ	6.911	0.001	.
1	A	45	PHE	CE2	130.97	0.035	.
1	A	45	PHE	CD2	131.539	0.065	.
1	A	45	PHE	C	175.856	0.000	.
1	A	46	VAL	N	118.269	0.037	.
1	A	46	VAL	H	9.168	0.005	.
1	A	46	VAL	CA	59.181	0.065	.
1	A	46	VAL	HA	5.747	0.009	.
1	A	46	VAL	CB	36.149	0.009	.
1	A	46	VAL	HB	1.752	0.007	.
1	A	46	VAL	HG11	0.794	0.009	.
1	A	46	VAL	HG12	0.794	0.009	.
1	A	46	VAL	HG13	0.794	0.009	.
1	A	46	VAL	HG21	0.746	0.008	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	46	VAL	HG22	0.746	0.008	.
1	A	46	VAL	HG23	0.746	0.008	.
1	A	46	VAL	CG1	21.423	0.042	.
1	A	46	VAL	CG2	21.629	0.033	.
1	A	46	VAL	C	173.156	0.000	.
1	A	47	ARG	N	122.361	0.043	.
1	A	47	ARG	H	8.64	0.005	.
1	A	47	ARG	CA	53.36	0.032	.
1	A	47	ARG	HA	5.647	0.007	.
1	A	47	ARG	CB	33.919	0.080	.
1	A	47	ARG	HB2	1.529	0.007	.
1	A	47	ARG	HB3	1.782	0.012	.
1	A	47	ARG	HG2	1.204	0.011	.
1	A	47	ARG	HG3	1.384	0.007	.
1	A	47	ARG	CD	44.878	0.000	.
1	A	47	ARG	HD2	2.674	0.013	.
1	A	47	ARG	NE	86.047	0.033	.
1	A	47	ARG	HE	7.73	0.007	.
1	A	47	ARG	C	174.957	0.000	.
1	A	48	ALA	N	127.463	0.057	.
1	A	48	ALA	H	8.29	0.009	.
1	A	48	ALA	CA	49.642	0.006	.
1	A	48	ALA	HA	5.49	0.008	.
1	A	48	ALA	HB1	1.149	0.007	.
1	A	48	ALA	HB2	1.149	0.007	.
1	A	48	ALA	HB3	1.149	0.007	.
1	A	48	ALA	CB	23.092	0.055	.
1	A	48	ALA	C	175.271	0.000	.
1	A	49	TYR	N	119.893	0.020	.
1	A	49	TYR	H	8.777	0.006	.
1	A	49	TYR	CA	55.954	0.046	.
1	A	49	TYR	HA	4.947	0.010	.
1	A	49	TYR	CB	40.523	0.033	.
1	A	49	TYR	HB2	2.327	0.009	.
1	A	49	TYR	HB3	1.934	0.013	.
1	A	49	TYR	HD1	6.466	0.011	.
1	A	49	TYR	HD2	6.466	0.011	.
1	A	49	TYR	HE1	6.22	0.013	.
1	A	49	TYR	HE2	6.22	0.013	.
1	A	49	TYR	CE2	116.978	0.003	.
1	A	49	TYR	CD2	132.534	0.046	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	49	TYR	C	171.969	0.000	.
1	A	50	ASN	N	125.67	0.044	.
1	A	50	ASN	H	8.121	0.003	.
1	A	50	ASN	CA	49.756	0.014	.
1	A	50	ASN	HA	4.367	0.010	.
1	A	50	ASN	CB	39.552	0.016	.
1	A	50	ASN	HB2	1.835	0.007	.
1	A	50	ASN	HB3	3.396	0.009	.
1	A	50	ASN	CG	176.533	0.000	.
1	A	50	ASN	ND2	113.217	0.054	.
1	A	50	ASN	HD21	7.684	0.008	.
1	A	50	ASN	HD22	6.335	0.003	.
1	A	50	ASN	C	172.008	0.000	.
1	A	51	ALA	N	124.71	0.036	.
1	A	51	ALA	H	7.702	0.007	.
1	A	51	ALA	CA	51.416	0.043	.
1	A	51	ALA	HA	4.252	0.011	.
1	A	51	ALA	HB1	1.284	0.007	.
1	A	51	ALA	HB2	1.284	0.007	.
1	A	51	ALA	HB3	1.284	0.007	.
1	A	51	ALA	CB	17.857	0.065	.
1	A	51	ALA	C	177.287	0.000	.
1	A	52	GLY	N	105.597	0.033	.
1	A	52	GLY	H	7.688	0.006	.
1	A	52	GLY	CA	44.226	0.006	.
1	A	52	GLY	HA2	4.093	0.013	.
1	A	52	GLY	HA3	3.705	0.008	.
1	A	52	GLY	C	171.542	0.000	.
1	A	53	ASN	N	110.82	0.018	.
1	A	53	ASN	H	7.878	0.004	.
1	A	53	ASN	CA	52.833	0.052	.
1	A	53	ASN	HA	4.778	0.010	.
1	A	53	ASN	CB	39.652	0.015	.
1	A	53	ASN	HB2	2.791	0.009	.
1	A	53	ASN	HB3	2.737	0.006	.
1	A	53	ASN	CG	177.542	0.000	.
1	A	53	ASN	ND2	112.231	0.055	.
1	A	53	ASN	HD21	6.825	0.004	.
1	A	53	ASN	HD22	7.536	0.004	.
1	A	53	ASN	C	175.07	0.000	.
1	A	54	SER	N	113.815	0.051	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	54	SER	H	7.701	0.007	.
1	A	54	SER	CA	56.466	0.016	.
1	A	54	SER	HA	4.621	0.006	.
1	A	54	SER	CB	65.198	0.017	.
1	A	54	SER	HB2	3.758	0.006	.
1	A	54	SER	HB3	3.753	0.009	.
1	A	54	SER	C	172.892	0.000	.
1	A	55	GLU	N	123.69	0.041	.
1	A	55	GLU	H	9.084	0.009	.
1	A	55	GLU	CA	58.32	0.004	.
1	A	55	GLU	HA	4.014	0.006	.
1	A	55	GLU	CB	30.098	0.016	.
1	A	55	GLU	HB2	1.878	0.010	.
1	A	55	GLU	HB3	1.781	0.007	.
1	A	55	GLU	CG	37.085	0.023	.
1	A	55	GLU	HG2	2.308	0.007	.
1	A	55	GLU	HG3	2.085	0.009	.
1	A	55	GLU	C	174.87	0.000	.
1	A	56	LEU	N	123.855	0.023	.
1	A	56	LEU	H	8.078	0.007	.
1	A	56	LEU	CA	53.855	0.061	.
1	A	56	LEU	HA	4.595	0.004	.
1	A	56	LEU	CB	47.006	0.052	.
1	A	56	LEU	HB2	1.213	0.012	.
1	A	56	LEU	HB3	1.557	0.008	.
1	A	56	LEU	CG	27.054	0.054	.
1	A	56	LEU	HG	0.525	0.009	.
1	A	56	LEU	HD11	0.525	0.009	.
1	A	56	LEU	HD12	0.525	0.009	.
1	A	56	LEU	HD13	0.525	0.009	.
1	A	56	LEU	HD21	0.739	0.011	.
1	A	56	LEU	HD22	0.739	0.011	.
1	A	56	LEU	HD23	0.739	0.011	.
1	A	56	LEU	CD1	27.057	0.053	.
1	A	56	LEU	CD2	23.358	0.050	.
1	A	56	LEU	C	173.291	0.000	.
1	A	57	ASP	N	123.122	0.042	.
1	A	57	ASP	H	8.096	0.003	.
1	A	57	ASP	CA	53.001	0.045	.
1	A	57	ASP	HA	5.407	0.012	.
1	A	57	ASP	CB	42.732	0.028	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	57	ASP	HB2	2.622	0.005	.
1	A	57	ASP	HB3	2.435	0.007	.
1	A	57	ASP	C	175.374	0.000	.
1	A	58	VAL	N	122.678	0.029	.
1	A	58	VAL	H	8.549	0.010	.
1	A	58	VAL	CA	59.63	0.006	.
1	A	58	VAL	HA	5.123	0.008	.
1	A	58	VAL	CB	35.204	0.016	.
1	A	58	VAL	HB	2.035	0.005	.
1	A	58	VAL	HG11	0.858	0.010	.
1	A	58	VAL	HG12	0.858	0.010	.
1	A	58	VAL	HG13	0.858	0.010	.
1	A	58	VAL	HG21	0.763	0.011	.
1	A	58	VAL	HG22	0.763	0.011	.
1	A	58	VAL	HG23	0.763	0.011	.
1	A	58	VAL	CG1	22.81	0.045	.
1	A	58	VAL	CG2	22.154	0.045	.
1	A	58	VAL	C	174.508	0.000	.
1	A	59	SER	N	120.51	0.038	.
1	A	59	SER	H	9.031	0.006	.
1	A	59	SER	CA	57.009	0.029	.
1	A	59	SER	HA	5.119	0.008	.
1	A	59	SER	CB	65.747	0.052	.
1	A	59	SER	HB2	3.696	0.009	.
1	A	59	SER	HB3	3.76	0.011	.
1	A	59	SER	C	173.1	0.000	.
1	A	60	VAL	N	122.436	0.051	.
1	A	60	VAL	H	8.571	0.004	.
1	A	60	VAL	CA	61.101	0.071	.
1	A	60	VAL	HA	3.918	0.007	.
1	A	60	VAL	CB	32.272	0.065	.
1	A	60	VAL	HB	1.627	0.011	.
1	A	60	VAL	HG11	0.177	0.009	.
1	A	60	VAL	HG12	0.177	0.009	.
1	A	60	VAL	HG13	0.177	0.009	.
1	A	60	VAL	HG21	0.437	0.009	.
1	A	60	VAL	HG22	0.437	0.009	.
1	A	60	VAL	HG23	0.437	0.009	.
1	A	60	VAL	CG1	21.084	0.022	.
1	A	60	VAL	CG2	20.764	0.036	.
1	A	60	VAL	C	174.674	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	61	GLY	N	115.605	0.018	.
1	A	61	GLY	H	8.655	0.003	.
1	A	61	GLY	CA	47.339	0.000	.
1	A	61	GLY	HA2	3.77	0.014	.
1	A	61	GLY	HA3	3.907	0.007	.
1	A	61	GLY	C	174.674	0.000	.
1	A	62	SER	CA	58.418	0.000	.
1	A	62	SER	HA	4.41	0.005	.
1	A	62	SER	CB	63.084	0.056	.
1	A	62	SER	HB2	4.057	0.005	.
1	A	62	SER	HB3	3.876	0.004	.
1	A	62	SER	C	173.984	0.000	.
1	A	63	THR	N	121.504	0.051	.
1	A	63	THR	H	8.079	0.006	.
1	A	63	THR	CA	63.102	0.056	.
1	A	63	THR	HA	4.255	0.007	.
1	A	63	THR	CB	69.232	0.059	.
1	A	63	THR	HB	3.997	0.007	.
1	A	63	THR	HG21	0.868	0.006	.
1	A	63	THR	HG22	0.868	0.006	.
1	A	63	THR	HG23	0.868	0.006	.
1	A	63	THR	HG1	0.861	0.012	.
1	A	63	THR	CG2	21.096	0.035	.
1	A	63	THR	C	172.781	0.000	.
1	A	64	SER	N	122.042	0.040	.
1	A	64	SER	H	8.597	0.011	.
1	A	64	SER	CA	57.247	0.094	.
1	A	64	SER	HA	4.889	0.010	.
1	A	64	SER	CB	65.193	0.022	.
1	A	64	SER	HB2	3.691	0.008	.
1	A	64	SER	HB3	3.757	0.010	.
1	A	64	SER	C	172.566	0.000	.
1	A	65	LEU	N	127.305	0.013	.
1	A	65	LEU	H	9.014	0.008	.
1	A	65	LEU	CA	53.556	0.040	.
1	A	65	LEU	HA	4.575	0.008	.
1	A	65	LEU	CB	41.387	0.033	.
1	A	65	LEU	HB2	1.686	0.011	.
1	A	65	LEU	HB3	1.242	0.011	.
1	A	65	LEU	CG	26.969	0.048	.
1	A	65	LEU	HG	1.387	0.010	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	65	LEU	HD11	0.695	0.008	.
1	A	65	LEU	HD12	0.695	0.008	.
1	A	65	LEU	HD13	0.695	0.008	.
1	A	65	LEU	HD21	0.865	0.007	.
1	A	65	LEU	HD22	0.865	0.007	.
1	A	65	LEU	HD23	0.865	0.007	.
1	A	65	LEU	CD1	25.515	0.054	.
1	A	65	LEU	CD2	24.527	0.073	.
1	A	65	LEU	C	174.079	0.000	.
1	A	66	ASN	N	118.176	0.021	.
1	A	66	ASN	H	8.147	0.004	.
1	A	66	ASN	CA	52.502	0.048	.
1	A	66	ASN	HA	5.195	0.011	.
1	A	66	ASN	CB	40.76	0.027	.
1	A	66	ASN	HB2	2.704	0.008	.
1	A	66	ASN	HB3	2.512	0.007	.
1	A	66	ASN	CG	176.251	0.000	.
1	A	66	ASN	ND2	109.711	0.039	.
1	A	66	ASN	HD21	7.384	0.003	.
1	A	66	ASN	HD22	6.584	0.002	.
1	A	66	ASN	C	175.35	0.000	.
1	A	67	ASP	N	118.525	0.032	.
1	A	67	ASP	H	9.09	0.005	.
1	A	67	ASP	CA	54.726	0.023	.
1	A	67	ASP	HA	4.016	0.006	.
1	A	67	ASP	CB	39.641	0.047	.
1	A	67	ASP	HB2	2.712	0.009	.
1	A	67	ASP	HB3	2.565	0.008	.
1	A	67	ASP	C	175.397	0.000	.
1	A	68	VAL	N	121.57	0.025	.
1	A	68	VAL	H	9.189	0.006	.
1	A	68	VAL	CA	63.403	0.026	.
1	A	68	VAL	HA	3.71	0.006	.
1	A	68	VAL	CB	31.215	0.063	.
1	A	68	VAL	HB	1.922	0.010	.
1	A	68	VAL	HG11	0.766	0.009	.
1	A	68	VAL	HG12	0.766	0.009	.
1	A	68	VAL	HG13	0.766	0.009	.
1	A	68	VAL	HG21	0.743	0.012	.
1	A	68	VAL	HG22	0.743	0.012	.
1	A	68	VAL	HG23	0.743	0.012	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	68	VAL	CG1	22.594	0.061	.
1	A	68	VAL	CG2	21.314	0.041	.
1	A	68	VAL	C	176.929	0.000	.
1	A	69	ALA	N	133.181	0.021	.
1	A	69	ALA	H	8.541	0.008	.
1	A	69	ALA	CA	51.476	0.063	.
1	A	69	ALA	HA	4.254	0.007	.
1	A	69	ALA	HB1	1.351	0.004	.
1	A	69	ALA	HB2	1.351	0.004	.
1	A	69	ALA	HB3	1.351	0.004	.
1	A	69	ALA	CB	18.099	0.066	.
1	A	69	ALA	C	176.929	0.000	.
1	A	70	PRO	CD	50.659	0.011	.
1	A	70	PRO	CA	64.067	0.012	.
1	A	70	PRO	HA	3.981	0.010	.
1	A	70	PRO	CB	32.092	0.036	.
1	A	70	PRO	HB2	1.781	0.009	.
1	A	70	PRO	HB3	2.091	0.012	.
1	A	70	PRO	CG	27.806	0.056	.
1	A	70	PRO	HG2	1.287	0.009	.
1	A	70	PRO	HG3	1.978	0.009	.
1	A	70	PRO	HD2	3.33	0.010	.
1	A	70	PRO	HD3	3.534	0.009	.
1	A	70	PRO	C	177.576	0.000	.
1	A	71	LEU	N	122.803	0.037	.
1	A	71	LEU	H	8.274	0.006	.
1	A	71	LEU	CA	56.84	0.019	.
1	A	71	LEU	HA	4.334	0.010	.
1	A	71	LEU	CB	38.629	0.020	.
1	A	71	LEU	HB2	2.104	0.012	.
1	A	71	LEU	HB3	1.733	0.011	.
1	A	71	LEU	CG	27.36	0.043	.
1	A	71	LEU	HG	1.47	0.007	.
1	A	71	LEU	HD11	0.884	0.007	.
1	A	71	LEU	HD12	0.884	0.007	.
1	A	71	LEU	HD13	0.884	0.007	.
1	A	71	LEU	HD21	0.8	0.009	.
1	A	71	LEU	HD22	0.8	0.009	.
1	A	71	LEU	HD23	0.8	0.009	.
1	A	71	LEU	CD1	25.613	0.030	.
1	A	71	LEU	CD2	22.776	0.073	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	71	LEU	C	176.299	0.000	.
1	A	72	GLY	N	109.43	0.035	.
1	A	72	GLY	H	8.514	0.008	.
1	A	72	GLY	CA	43.886	0.010	.
1	A	72	GLY	HA2	4.606	0.010	.
1	A	72	GLY	HA3	3.608	0.011	.
1	A	72	GLY	C	171.268	0.000	.
1	A	73	SER	N	108.857	0.013	.
1	A	73	SER	H	8.31	0.002	.
1	A	73	SER	CA	56.417	0.045	.
1	A	73	SER	HA	5.644	0.008	.
1	A	73	SER	CB	67.665	0.057	.
1	A	73	SER	HB2	3.762	0.013	.
1	A	73	SER	HB3	3.877	0.010	.
1	A	73	SER	C	174.787	0.000	.
1	A	74	SER	N	116.653	0.017	.
1	A	74	SER	H	8.638	0.006	.
1	A	74	SER	CA	56.816	0.038	.
1	A	74	SER	HA	4.926	0.010	.
1	A	74	SER	CB	67.602	0.035	.
1	A	74	SER	HB2	3.708	0.013	.
1	A	74	SER	HB3	3.704	0.010	.
1	A	74	SER	C	174.335	0.000	.
1	A	75	ASP	N	117.29	0.059	.
1	A	75	ASP	H	8.771	0.005	.
1	A	75	ASP	CA	52.841	0.053	.
1	A	75	ASP	HA	4.811	0.008	.
1	A	75	ASP	CB	41.446	0.054	.
1	A	75	ASP	HB2	2.705	0.008	.
1	A	75	ASP	HB3	2.606	0.009	.
1	A	75	ASP	C	178.136	0.000	.
1	A	76	PHE	N	119.401	0.018	.
1	A	76	PHE	H	9.338	0.005	.
1	A	76	PHE	CA	58.942	0.000	.
1	A	76	PHE	HA	4.741	0.008	.
1	A	76	PHE	CB	41.414	0.054	.
1	A	76	PHE	HB2	3.106	0.012	.
1	A	76	PHE	HB3	2.98	0.009	.
1	A	76	PHE	HD1	7.195	0.013	.
1	A	76	PHE	HD2	7.195	0.013	.
1	A	76	PHE	HE1	7.441	0.005	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	76	PHE	HE2	7.441	0.005	.
1	A	76	PHE	CD1	132.249	0.000	.
1	A	76	PHE	CE1	132.088	0.025	.
1	A	76	PHE	CZ	129.031	0.000	.
1	A	76	PHE	HZ	6.957	0.003	.
1	A	76	PHE	C	176.883	0.000	.
1	A	77	LYS	N	122.964	0.016	.
1	A	77	LYS	H	9.194	0.010	.
1	A	77	LYS	CA	55.376	0.010	.
1	A	77	LYS	HA	4.742	0.012	.
1	A	77	LYS	CB	35.799	0.013	.
1	A	77	LYS	HB2	1.743	0.010	.
1	A	77	LYS	HB3	1.405	0.007	.
1	A	77	LYS	CG	26.384	0.060	.
1	A	77	LYS	HG2	1.405	0.009	.
1	A	77	LYS	HG3	1.405	0.009	.
1	A	77	LYS	CD	29.527	0.029	.
1	A	77	LYS	HD2	1.647	0.010	.
1	A	77	LYS	HD3	1.544	0.011	.
1	A	77	LYS	CE	42.135	0.063	.
1	A	77	LYS	HE2	3.029	0.009	.
1	A	77	LYS	HE3	2.979	0.006	.
1	A	77	LYS	C	175.125	0.000	.
1	A	78	PHE	N	116.858	0.023	.
1	A	78	PHE	H	7.163	0.007	.
1	A	78	PHE	CA	54.03	0.025	.
1	A	78	PHE	HA	5.506	0.011	.
1	A	78	PHE	CB	41.23	0.023	.
1	A	78	PHE	HB2	2.516	0.007	.
1	A	78	PHE	HB3	2.453	0.011	.
1	A	78	PHE	HD1	7.056	0.009	.
1	A	78	PHE	HD2	7.056	0.009	.
1	A	78	PHE	HE1	7.333	0.015	.
1	A	78	PHE	HE2	7.333	0.015	.
1	A	78	PHE	CD1	132.739	0.070	.
1	A	78	PHE	CE1	131.435	0.024	.
1	A	78	PHE	CZ	130.192	0.000	.
1	A	78	PHE	HZ	7.237	0.014	.
1	A	78	PHE	C	174.393	0.000	.
1	A	79	LEU	N	121.025	0.023	.
1	A	79	LEU	H	8.799	0.005	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	79	LEU	CA	54.538	0.037	.
1	A	79	LEU	HA	4.624	0.007	.
1	A	79	LEU	CB	40.659	0.023	.
1	A	79	LEU	HB2	1.581	0.007	.
1	A	79	LEU	HB3	1.518	0.009	.
1	A	79	LEU	CG	26.875	0.043	.
1	A	79	LEU	HG	1.389	0.006	.
1	A	79	LEU	HD11	0.478	0.011	.
1	A	79	LEU	HD12	0.478	0.011	.
1	A	79	LEU	HD13	0.478	0.011	.
1	A	79	LEU	HD21	0.162	0.007	.
1	A	79	LEU	HD22	0.162	0.007	.
1	A	79	LEU	HD23	0.162	0.007	.
1	A	79	LEU	CD1	25.532	0.052	.
1	A	79	LEU	CD2	26.901	0.011	.
1	A	79	LEU	C	174.393	0.000	.
1	A	80	PRO	CD	49.84	0.037	.
1	A	80	PRO	CA	61.685	0.017	.
1	A	80	PRO	HA	4.532	0.009	.
1	A	80	PRO	CB	30.427	0.051	.
1	A	80	PRO	HB2	2.394	0.006	.
1	A	80	PRO	HB3	1.713	0.008	.
1	A	80	PRO	HD2	3.74	0.012	.
1	A	80	PRO	HD3	3.556	0.008	.
1	A	81	PRO	CD	50.662	0.035	.
1	A	81	PRO	CA	62.983	0.052	.
1	A	81	PRO	HA	4.252	0.009	.
1	A	81	PRO	CB	32.12	0.025	.
1	A	81	PRO	HB2	1.781	0.009	.
1	A	81	PRO	HB3	2.079	0.010	.
1	A	81	PRO	CG	27.869	0.051	.
1	A	81	PRO	HG2	2.123	0.008	.
1	A	81	PRO	HG3	1.984	0.007	.
1	A	81	PRO	HD2	3.563	0.011	.
1	A	81	PRO	HD3	3.327	0.011	.
1	A	81	PRO	C	175.364	0.000	.
1	A	82	GLY	N	107.059	0.024	.
1	A	82	GLY	H	8.476	0.002	.
1	A	82	GLY	CA	44.246	0.015	.
1	A	82	GLY	HA2	4.123	0.011	.
1	A	82	GLY	HA3	3.709	0.008	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	82	GLY	C	171.59	0.000	.
1	A	83	SER	N	115.746	0.039	.
1	A	83	SER	H	8.01	0.003	.
1	A	83	SER	CA	57.518	0.042	.
1	A	83	SER	HA	5.239	0.006	.
1	A	83	SER	CB	63.523	0.046	.
1	A	83	SER	HB2	3.72	0.008	.
1	A	83	SER	HB3	3.544	0.011	.
1	A	83	SER	C	173.495	0.000	.
1	A	84	TYR	N	120.903	0.033	.
1	A	84	TYR	H	8.741	0.004	.
1	A	84	TYR	CA	56.315	0.019	.
1	A	84	TYR	HA	4.79	0.015	.
1	A	84	TYR	CB	44.213	0.041	.
1	A	84	TYR	HB2	2.851	0.010	.
1	A	84	TYR	HB3	2.098	0.008	.
1	A	84	TYR	HD1	6.743	0.006	.
1	A	84	TYR	HD2	6.743	0.006	.
1	A	84	TYR	HE1	6.621	0.003	.
1	A	84	TYR	HE2	6.621	0.003	.
1	A	84	TYR	CD1	133.319	0.037	.
1	A	84	TYR	CE1	117.286	0.000	.
1	A	84	TYR	C	175.463	0.000	.
1	A	85	THR	N	118.877	0.041	.
1	A	85	THR	H	9.04	0.004	.
1	A	85	THR	CA	62.836	0.067	.
1	A	85	THR	HA	4.519	0.008	.
1	A	85	THR	CB	68.394	0.054	.
1	A	85	THR	HB	4.003	0.006	.
1	A	85	THR	HG21	1.031	0.006	.
1	A	85	THR	HG22	1.031	0.006	.
1	A	85	THR	HG23	1.031	0.006	.
1	A	85	THR	CG2	22.222	0.043	.
1	A	85	THR	C	174.237	0.000	.
1	A	86	ALA	N	130.936	0.021	.
1	A	86	ALA	H	9.103	0.006	.
1	A	86	ALA	CA	50.749	0.043	.
1	A	86	ALA	HA	4.798	0.012	.
1	A	86	ALA	HB1	1.222	0.009	.
1	A	86	ALA	HB2	1.222	0.009	.
1	A	86	ALA	HB3	1.222	0.009	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	86	ALA	CB	20.467	0.032	.
1	A	86	ALA	C	175.311	0.000	.
1	A	87	GLN	N	123.37	0.052	.
1	A	87	GLN	H	9.068	0.010	.
1	A	87	GLN	CA	54.527	0.029	.
1	A	87	GLN	HA	4.644	0.008	.
1	A	87	GLN	CB	28.93	0.015	.
1	A	87	GLN	HB2	2.101	0.006	.
1	A	87	GLN	HB3	1.915	0.010	.
1	A	87	GLN	CG	33.029	0.072	.
1	A	87	GLN	HG2	2.236	0.010	.
1	A	87	GLN	HG3	2.236	0.010	.
1	A	87	GLN	CD	180.027	0.000	.
1	A	87	GLN	NE2	111.205	0.028	.
1	A	87	GLN	HE21	6.556	0.003	.
1	A	87	GLN	HE22	7.299	0.004	.
1	A	87	GLN	C	174.526	0.000	.
1	A	88	VAL	N	127.008	0.034	.
1	A	88	VAL	H	8.909	0.008	.
1	A	88	VAL	CA	60.18	0.043	.
1	A	88	VAL	HA	4.261	0.007	.
1	A	88	VAL	CB	31.105	0.002	.
1	A	88	VAL	HB	2.032	0.009	.
1	A	88	VAL	HG11	0.728	0.012	.
1	A	88	VAL	HG12	0.728	0.012	.
1	A	88	VAL	HG13	0.728	0.012	.
1	A	88	VAL	HG21	0.762	0.009	.
1	A	88	VAL	HG22	0.762	0.009	.
1	A	88	VAL	HG23	0.762	0.009	.
1	A	88	VAL	CG1	21.104	0.046	.
1	A	88	VAL	CG2	22.147	0.048	.
1	A	88	VAL	C	175.776	0.000	.
1	A	89	GLY	N	118.064	0.021	.
1	A	89	GLY	H	8.645	0.006	.
1	A	89	GLY	CA	47.567	0.046	.
1	A	89	GLY	HA2	3.991	0.010	.
1	A	89	GLY	HA3	3.992	0.011	.
1	A	89	GLY	C	175.081	0.000	.
1	A	90	GLN	N	125.774	0.044	.
1	A	90	GLN	H	9.051	0.012	.
1	A	90	GLN	CA	56.129	0.062	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	90	GLN	HA	4.323	0.006	.
1	A	90	GLN	CB	28.946	0.011	.
1	A	90	GLN	HB2	2.363	0.006	.
1	A	90	GLN	HB3	1.918	0.003	.
1	A	90	GLN	CG	34.218	0.015	.
1	A	90	GLN	HG2	2.365	0.009	.
1	A	90	GLN	HG3	2.369	0.008	.
1	A	90	GLN	CD	180.515	0.000	.
1	A	90	GLN	NE2	113.409	0.017	.
1	A	90	GLN	HE21	7.471	0.003	.
1	A	90	GLN	HE22	6.826	0.004	.
1	A	90	GLN	C	175.461	0.000	.
1	A	91	GLN	N	118.051	0.014	.
1	A	91	GLN	H	7.673	0.002	.
1	A	91	GLN	CA	54.998	0.000	.
1	A	91	GLN	HA	4.662	0.009	.
1	A	91	GLN	CB	32.918	0.046	.
1	A	91	GLN	HB2	2.003	0.007	.
1	A	91	GLN	HB3	2.113	0.014	.
1	A	91	GLN	CG	34.873	0.029	.
1	A	91	GLN	HG2	2.335	0.012	.
1	A	91	GLN	HG3	2.335	0.012	.
1	A	91	GLN	CD	180.277	0.000	.
1	A	91	GLN	NE2	113.568	0.021	.
1	A	91	GLN	HE21	7.056	0.001	.
1	A	91	GLN	HE22	7.695	0.006	.
1	A	91	GLN	C	173.927	0.000	.
1	A	92	SER	N	117.181	0.030	.
1	A	92	SER	H	8.612	0.008	.
1	A	92	SER	CA	56.999	0.026	.
1	A	92	SER	HA	5.327	0.007	.
1	A	92	SER	CB	65.261	0.030	.
1	A	92	SER	HB2	3.674	0.012	.
1	A	92	SER	HB3	3.676	0.012	.
1	A	92	SER	C	173.779	0.000	.
1	A	93	LEU	N	123.349	0.014	.
1	A	93	LEU	H	8.958	0.007	.
1	A	93	LEU	CA	52.595	0.030	.
1	A	93	LEU	HA	4.952	0.007	.
1	A	93	LEU	CB	46.041	0.046	.
1	A	93	LEU	HB2	1.616	0.008	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	93	LEU	HB3	1.269	0.009	.
1	A	93	LEU	CG	26.798	0.072	.
1	A	93	LEU	HG	1.278	0.009	.
1	A	93	LEU	HD11	0.563	0.008	.
1	A	93	LEU	HD12	0.563	0.008	.
1	A	93	LEU	HD13	0.563	0.008	.
1	A	93	LEU	HD21	0.893	0.009	.
1	A	93	LEU	HD22	0.893	0.009	.
1	A	93	LEU	HD23	0.893	0.009	.
1	A	93	LEU	CD1	26.232	0.029	.
1	A	93	LEU	CD2	24.055	0.045	.
1	A	93	LEU	C	173.779	0.000	.
1	A	94	PRO	CD	51.317	0.027	.
1	A	94	PRO	CA	62.776	0.052	.
1	A	94	PRO	HA	5.002	0.010	.
1	A	94	PRO	CB	31.762	0.030	.
1	A	94	PRO	HB2	2.329	0.009	.
1	A	94	PRO	HB3	1.944	0.015	.
1	A	94	PRO	CG	27.762	0.045	.
1	A	94	PRO	HG2	1.96	0.010	.
1	A	94	PRO	HG3	2.184	0.008	.
1	A	94	PRO	HD2	3.763	0.009	.
1	A	94	PRO	HD3	3.86	0.012	.
1	A	94	PRO	C	176.866	0.000	.
1	A	95	VAL	N	115.469	0.025	.
1	A	95	VAL	H	9.101	0.005	.
1	A	95	VAL	CA	58.915	0.055	.
1	A	95	VAL	HA	4.727	0.013	.
1	A	95	VAL	CB	36.168	0.043	.
1	A	95	VAL	HB	1.849	0.008	.
1	A	95	VAL	HG11	0.833	0.010	.
1	A	95	VAL	HG12	0.833	0.010	.
1	A	95	VAL	HG13	0.833	0.010	.
1	A	95	VAL	HG21	0.72	0.011	.
1	A	95	VAL	HG22	0.72	0.011	.
1	A	95	VAL	HG23	0.72	0.011	.
1	A	95	VAL	CG1	23.629	0.044	.
1	A	95	VAL	CG2	19.852	0.030	.
1	A	95	VAL	C	173.708	0.000	.
1	A	96	LYS	N	125.032	0.020	.
1	A	96	LYS	H	7.852	0.004	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	96	LYS	CA	55.505	0.049	.
1	A	96	LYS	HA	4.747	0.012	.
1	A	96	LYS	CB	33.859	0.031	.
1	A	96	LYS	HB2	1.674	0.009	.
1	A	96	LYS	HB3	1.53	0.010	.
1	A	96	LYS	CG	25.156	0.039	.
1	A	96	LYS	HG2	1.168	0.007	.
1	A	96	LYS	HG3	1.134	0.006	.
1	A	96	LYS	CD	28.829	0.050	.
1	A	96	LYS	HD2	1.673	0.010	.
1	A	96	LYS	HD3	1.54	0.012	.
1	A	96	LYS	CE	41.82	0.040	.
1	A	96	LYS	HE2	2.893	0.009	.
1	A	96	LYS	HE3	2.929	0.005	.
1	A	96	LYS	C	173.769	0.000	.
1	A	97	LEU	N	124.291	0.027	.
1	A	97	LEU	H	8.791	0.003	.
1	A	97	LEU	CA	52.53	0.052	.
1	A	97	LEU	HA	4.388	0.008	.
1	A	97	LEU	CB	42.403	0.042	.
1	A	97	LEU	HB2	1.139	0.012	.
1	A	97	LEU	HB3	1.796	0.011	.
1	A	97	LEU	CG	27.356	0.056	.
1	A	97	LEU	HG	1.434	0.012	.
1	A	97	LEU	HD11	0.539	0.010	.
1	A	97	LEU	HD12	0.539	0.010	.
1	A	97	LEU	HD13	0.539	0.010	.
1	A	97	LEU	HD21	-0.04	0.007	.
1	A	97	LEU	HD22	-0.04	0.007	.
1	A	97	LEU	HD23	-0.04	0.007	.
1	A	97	LEU	CD1	27.233	0.036	.
1	A	97	LEU	CD2	22.5	0.026	.
1	A	97	LEU	C	176.102	0.000	.
1	A	98	ASP	N	126.305	0.033	.
1	A	98	ASP	H	8.879	0.006	.
1	A	98	ASP	CA	52.75	0.037	.
1	A	98	ASP	HA	5.045	0.011	.
1	A	98	ASP	CB	40.29	0.025	.
1	A	98	ASP	HB2	2.615	0.011	.
1	A	98	ASP	HB3	2.704	0.004	.
1	A	98	ASP	C	176.102	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	99	PRO	CD	50.388	0.026	.
1	A	99	PRO	CA	63.307	0.045	.
1	A	99	PRO	HA	4.263	0.009	.
1	A	99	PRO	CB	32.412	0.031	.
1	A	99	PRO	HB2	2.368	0.010	.
1	A	99	PRO	HB3	2.368	0.010	.
1	A	99	PRO	CG	27.569	0.000	.
1	A	99	PRO	HG2	1.842	0.013	.
1	A	99	PRO	HG3	1.842	0.013	.
1	A	99	PRO	HD2	3.673	0.010	.
1	A	99	PRO	HD3	3.802	0.004	.
1	A	99	PRO	C	178.365	0.000	.
1	A	100	ASP	N	118.986	0.029	.
1	A	100	ASP	H	7.723	0.004	.
1	A	100	ASP	CA	55.634	0.008	.
1	A	100	ASP	HA	4.485	0.006	.
1	A	100	ASP	CB	39.993	0.015	.
1	A	100	ASP	HB2	2.985	0.009	.
1	A	100	ASP	HB3	2.757	0.007	.
1	A	100	ASP	C	174.388	0.000	.
1	A	101	SER	N	112.417	0.030	.
1	A	101	SER	H	7.1	0.007	.
1	A	101	SER	CA	58.728	0.019	.
1	A	101	SER	HA	4.847	0.008	.
1	A	101	SER	CB	66.266	0.000	.
1	A	101	SER	HB2	4.036	0.009	.
1	A	101	SER	HB3	3.664	0.010	.
1	A	101	SER	C	170.479	0.000	.
1	A	102	TYR	N	122.245	0.062	.
1	A	102	TYR	H	8.602	0.005	.
1	A	102	TYR	CA	56.503	0.017	.
1	A	102	TYR	HA	5.232	0.010	.
1	A	102	TYR	CB	40.621	0.006	.
1	A	102	TYR	HB2	3.063	0.010	.
1	A	102	TYR	HB3	2.209	0.014	.
1	A	102	TYR	HD1	5.847	0.015	.
1	A	102	TYR	HD2	5.847	0.015	.
1	A	102	TYR	HE1	5.817	0.014	.
1	A	102	TYR	HE2	5.817	0.014	.
1	A	102	TYR	CD1	132.051	0.011	.
1	A	102	TYR	CE1	117.497	0.011	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	102	TYR	C	176.044	0.000	.
1	A	103	TYR	N	117.741	0.024	.
1	A	103	TYR	H	8.942	0.006	.
1	A	103	TYR	CA	57.138	0.009	.
1	A	103	TYR	HA	5.382	0.008	.
1	A	103	TYR	CB	44.867	0.037	.
1	A	103	TYR	HB2	2.932	0.007	.
1	A	103	TYR	HB3	2.764	0.010	.
1	A	103	TYR	HD1	7.016	0.010	.
1	A	103	TYR	HD2	7.016	0.010	.
1	A	103	TYR	HE1	7.188	0.010	.
1	A	103	TYR	HE2	7.188	0.010	.
1	A	103	TYR	CE2	115.223	0.000	.
1	A	103	TYR	CD2	132.0	0.010	.
1	A	103	TYR	C	174.5	0.000	.
1	A	104	THR	N	119.901	0.009	.
1	A	104	THR	H	9.809	0.004	.
1	A	104	THR	CA	60.834	0.032	.
1	A	104	THR	HA	4.706	0.010	.
1	A	104	THR	CB	70.834	0.007	.
1	A	104	THR	HB	4.249	0.007	.
1	A	104	THR	HG21	0.762	0.008	.
1	A	104	THR	HG22	0.762	0.008	.
1	A	104	THR	HG23	0.762	0.008	.
1	A	104	THR	CG2	23.889	0.048	.
1	A	104	THR	C	174.129	0.000	.
1	A	105	LEU	N	129.229	0.025	.
1	A	105	LEU	H	9.462	0.010	.
1	A	105	LEU	CA	53.895	0.030	.
1	A	105	LEU	HA	5.035	0.007	.
1	A	105	LEU	CB	43.23	0.038	.
1	A	105	LEU	HB2	1.517	0.009	.
1	A	105	LEU	HB3	1.202	0.012	.
1	A	105	LEU	CG	27.588	0.064	.
1	A	105	LEU	HG	1.421	0.010	.
1	A	105	LEU	HD11	0.646	0.009	.
1	A	105	LEU	HD12	0.646	0.009	.
1	A	105	LEU	HD13	0.646	0.009	.
1	A	105	LEU	HD21	0.561	0.009	.
1	A	105	LEU	HD22	0.561	0.009	.
1	A	105	LEU	HD23	0.561	0.009	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	105	LEU	CD1	25.713	0.058	.
1	A	105	LEU	CD2	26.242	0.039	.
1	A	105	LEU	C	174.692	0.000	.
1	A	106	VAL	N	123.99	0.064	.
1	A	106	VAL	H	9.163	0.005	.
1	A	106	VAL	CA	61.247	0.053	.
1	A	106	VAL	HA	4.777	0.010	.
1	A	106	VAL	CB	34.74	0.033	.
1	A	106	VAL	HB	1.898	0.011	.
1	A	106	VAL	HG11	1.057	0.011	.
1	A	106	VAL	HG12	1.057	0.011	.
1	A	106	VAL	HG13	1.057	0.011	.
1	A	106	VAL	HG21	0.762	0.005	.
1	A	106	VAL	HG22	0.762	0.005	.
1	A	106	VAL	HG23	0.762	0.005	.
1	A	106	VAL	CG1	23.605	0.047	.
1	A	106	VAL	CG2	20.625	0.046	.
1	A	106	VAL	C	176.128	0.000	.
1	A	107	SER	N	119.57	0.028	.
1	A	107	SER	H	7.79	0.005	.
1	A	107	SER	CA	55.409	0.010	.
1	A	107	SER	HA	4.633	0.006	.
1	A	107	SER	CB	64.783	0.015	.
1	A	107	SER	HB2	3.513	0.008	.
1	A	107	SER	HB3	3.234	0.005	.
1	A	107	SER	C	173.183	0.000	.
1	A	108	GLN	N	124.319	0.027	.
1	A	108	GLN	H	8.953	0.006	.
1	A	108	GLN	CA	52.298	0.024	.
1	A	108	GLN	HA	4.776	0.007	.
1	A	108	GLN	CB	30.533	0.031	.
1	A	108	GLN	HB2	1.719	0.010	.
1	A	108	GLN	HB3	1.95	0.011	.
1	A	108	GLN	CG	33.088	0.041	.
1	A	108	GLN	HG2	2.241	0.006	.
1	A	108	GLN	HG3	2.111	0.008	.
1	A	108	GLN	CD	179.485	0.000	.
1	A	108	GLN	NE2	111.67	0.036	.
1	A	108	GLN	HE21	7.261	0.002	.
1	A	108	GLN	HE22	7.383	0.006	.
1	A	108	GLN	C	173.183	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	109	PRO	CD	50.665	0.030	.
1	A	109	PRO	CA	63.48	0.024	.
1	A	109	PRO	HA	4.315	0.011	.
1	A	109	PRO	CB	31.49	0.046	.
1	A	109	PRO	HB2	2.249	0.008	.
1	A	109	PRO	HB3	1.913	0.005	.
1	A	109	PRO	CG	27.902	0.075	.
1	A	109	PRO	HG2	2.112	0.011	.
1	A	109	PRO	HG3	2.112	0.011	.
1	A	109	PRO	HD2	3.322	0.006	.
1	A	109	PRO	HD3	3.569	0.007	.
1	A	110	GLY	HA2	4.268	0.000	.
1	A	110	GLY	HA3	4.268	0.000	.
1	A	111	GLY	CA	43.968	0.068	.
1	A	111	GLY	HA2	4.486	0.010	.
1	A	111	GLY	HA3	3.618	0.004	.
1	A	111	GLY	C	172.908	0.000	.
1	A	112	LYS	N	121.676	0.031	.
1	A	112	LYS	H	8.462	0.002	.
1	A	112	LYS	CA	54.491	0.062	.
1	A	112	LYS	HA	4.629	0.008	.
1	A	112	LYS	CB	32.238	0.043	.
1	A	112	LYS	HB2	1.9	0.009	.
1	A	112	LYS	HB3	1.723	0.009	.
1	A	112	LYS	CG	25.085	0.061	.
1	A	112	LYS	HG2	1.571	0.010	.
1	A	112	LYS	HG3	1.571	0.010	.
1	A	112	LYS	CD	28.931	0.000	.
1	A	112	LYS	HD2	2.1	0.006	.
1	A	112	LYS	HD3	2.17	0.000	.
1	A	113	PRO	CD	49.924	0.052	.
1	A	113	PRO	CA	62.451	0.056	.
1	A	113	PRO	HA	5.086	0.009	.
1	A	113	PRO	CB	32.217	0.030	.
1	A	113	PRO	HB2	2.176	0.009	.
1	A	113	PRO	HB3	1.717	0.010	.
1	A	113	PRO	CG	27.872	0.052	.
1	A	113	PRO	HG2	1.873	0.010	.
1	A	113	PRO	HG3	1.831	0.007	.
1	A	113	PRO	HD2	3.72	0.007	.
1	A	113	PRO	HD3	3.72	0.007	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	113	PRO	C	174.578	0.000	.
1	A	114	GLN	N	114.988	0.008	.
1	A	114	GLN	H	8.022	0.002	.
1	A	114	GLN	CA	54.643	0.047	.
1	A	114	GLN	HA	4.666	0.005	.
1	A	114	GLN	CB	34.145	0.056	.
1	A	114	GLN	HB2	1.753	0.011	.
1	A	114	GLN	HB3	1.996	0.011	.
1	A	114	GLN	CG	34.201	0.026	.
1	A	114	GLN	HG2	2.263	0.008	.
1	A	114	GLN	HG3	2.298	0.007	.
1	A	114	GLN	CD	180.637	0.000	.
1	A	114	GLN	NE2	112.829	0.018	.
1	A	114	GLN	HE21	6.83	0.002	.
1	A	114	GLN	HE22	7.57	0.001	.
1	A	114	GLN	C	173.088	0.000	.
1	A	115	LEU	N	125.764	0.013	.
1	A	115	LEU	H	8.895	0.006	.
1	A	115	LEU	CA	54.345	0.015	.
1	A	115	LEU	HA	4.738	0.014	.
1	A	115	LEU	CB	43.468	0.028	.
1	A	115	LEU	HB2	2.093	0.009	.
1	A	115	LEU	HB3	1.136	0.011	.
1	A	115	LEU	CG	26.324	0.042	.
1	A	115	LEU	HG	0.672	0.008	.
1	A	115	LEU	HD11	0.67	0.009	.
1	A	115	LEU	HD12	0.67	0.009	.
1	A	115	LEU	HD13	0.67	0.009	.
1	A	115	LEU	HD21	0.61	0.008	.
1	A	115	LEU	HD22	0.61	0.008	.
1	A	115	LEU	HD23	0.61	0.008	.
1	A	115	LEU	CD1	26.295	0.038	.
1	A	115	LEU	CD2	24.291	0.025	.
1	A	115	LEU	C	175.335	0.000	.
1	A	116	VAL	N	131.224	0.034	.
1	A	116	VAL	H	9.509	0.007	.
1	A	116	VAL	CA	61.679	0.056	.
1	A	116	VAL	HA	4.435	0.012	.
1	A	116	VAL	CB	33.656	0.014	.
1	A	116	VAL	HB	2.411	0.007	.
1	A	116	VAL	HG11	1.036	0.008	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	116	VAL	HG12	1.036	0.008	.
1	A	116	VAL	HG13	1.036	0.008	.
1	A	116	VAL	HG21	0.902	0.013	.
1	A	116	VAL	HG22	0.902	0.013	.
1	A	116	VAL	HG23	0.902	0.013	.
1	A	116	VAL	CG1	22.632	0.042	.
1	A	116	VAL	CG2	22.474	0.043	.
1	A	116	VAL	C	175.453	0.000	.
1	A	117	ALA	N	130.469	0.012	.
1	A	117	ALA	H	8.926	0.007	.
1	A	117	ALA	CA	53.002	0.054	.
1	A	117	ALA	HA	4.328	0.009	.
1	A	117	ALA	HB1	1.434	0.006	.
1	A	117	ALA	HB2	1.434	0.006	.
1	A	117	ALA	HB3	1.434	0.006	.
1	A	117	ALA	CB	19.197	0.053	.
1	A	117	ALA	C	177.022	0.000	.
1	A	118	GLU	N	120.762	0.035	.
1	A	118	GLU	H	7.995	0.004	.
1	A	118	GLU	CA	51.198	0.034	.
1	A	118	GLU	HA	4.788	0.011	.
1	A	118	GLU	CB	29.974	0.000	.
1	A	118	GLU	HB2	2.744	0.012	.
1	A	118	GLU	HB3	2.744	0.012	.
1	A	118	GLU	C	177.022	0.000	.
1	A	119	PRO	CD	49.58	0.029	.
1	A	119	PRO	HA	4.507	0.015	.
1	A	119	PRO	CB	32.404	0.018	.
1	A	119	PRO	HB2	2.369	0.014	.
1	A	119	PRO	HB3	2.369	0.014	.
1	A	119	PRO	CG	27.727	0.020	.
1	A	119	PRO	HG2	1.692	0.010	.
1	A	119	PRO	HG3	1.692	0.010	.
1	A	119	PRO	HD2	3.391	0.011	.
1	A	119	PRO	HD3	2.741	0.008	.
1	A	120	PRO	CD	50.491	0.019	.
1	A	120	PRO	CA	62.788	0.042	.
1	A	120	PRO	HA	4.17	0.007	.
1	A	120	PRO	CB	32.776	0.023	.
1	A	120	PRO	HB2	1.682	0.010	.
1	A	120	PRO	HB3	1.98	0.009	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	120	PRO	HD2	3.646	0.011	.
1	A	120	PRO	HD3	3.773	0.006	.
1	A	121	PHE	N	115.446	0.038	.
1	A	121	PHE	H	8.504	0.006	.
1	A	121	PHE	CA	56.501	0.017	.
1	A	121	PHE	HA	4.723	0.004	.
1	A	121	PHE	CB	41.642	0.032	.
1	A	121	PHE	HB2	2.714	0.005	.
1	A	121	PHE	HB3	2.535	0.010	.
1	A	121	PHE	HD1	6.753	0.000	.
1	A	121	PHE	HD2	6.753	0.000	.
1	A	121	PHE	HE1	7.199	0.005	.
1	A	121	PHE	HE2	7.199	0.005	.
1	A	121	PHE	CD1	130.301	0.000	.
1	A	121	PHE	CE1	131.954	0.000	.
1	A	122	LYS	N	118.067	0.000	.
1	A	122	LYS	H	7.674	0.000	.
1	A	122	LYS	CA	55.174	0.005	.
1	A	122	LYS	HA	4.171	0.002	.
1	A	122	LYS	CB	33.299	0.024	.
1	A	122	LYS	HB2	1.441	0.007	.
1	A	122	LYS	HB3	1.72	0.010	.
1	A	122	LYS	CG	24.701	0.039	.
1	A	122	LYS	HG2	1.133	0.012	.
1	A	122	LYS	HG3	1.134	0.012	.
1	A	122	LYS	CD	28.829	0.059	.
1	A	122	LYS	HD2	1.538	0.010	.
1	A	122	LYS	HD3	1.538	0.010	.
1	A	122	LYS	CE	41.713	0.009	.
1	A	122	LYS	HE2	2.837	0.007	.
1	A	122	LYS	HE3	2.837	0.007	.
1	A	122	LYS	C	174.857	0.000	.
1	A	123	ASN	N	118.763	0.027	.
1	A	123	ASN	H	6.093	0.004	.
1	A	123	ASN	CA	52.829	0.013	.
1	A	123	ASN	HA	4.304	0.009	.
1	A	123	ASN	CB	39.509	0.004	.
1	A	123	ASN	HB2	2.508	0.002	.
1	A	123	ASN	HB3	2.184	0.003	.
1	A	123	ASN	CG	177.092	0.000	.
1	A	123	ASN	ND2	114.051	0.031	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	123	ASN	HD21	7.872	0.007	.
1	A	123	ASN	HD22	6.911	0.003	.
1	A	123	ASN	C	174.421	0.000	.
1	A	213	PRO	CD	50.11	0.018	.
1	A	213	PRO	CA	62.799	0.053	.
1	A	213	PRO	HA	4.51	0.003	.
1	A	213	PRO	CB	31.769	0.025	.
1	A	213	PRO	HB2	2.33	0.004	.
1	A	213	PRO	HB3	1.955	0.013	.
1	A	213	PRO	CG	27.875	0.010	.
1	A	213	PRO	HG2	2.146	0.008	.
1	A	213	PRO	HG3	2.144	0.009	.
1	A	213	PRO	HD2	3.757	0.005	.
1	A	213	PRO	HD3	3.463	0.011	.
1	A	213	PRO	C	176.277	0.000	.
1	A	214	VAL	N	120.082	0.010	.
1	A	214	VAL	H	8.149	0.002	.
1	A	214	VAL	CA	61.584	0.070	.
1	A	214	VAL	HA	4.135	0.010	.
1	A	214	VAL	CB	33.202	0.015	.
1	A	214	VAL	HB	2.032	0.007	.
1	A	214	VAL	HG11	0.889	0.012	.
1	A	214	VAL	HG12	0.889	0.012	.
1	A	214	VAL	HG13	0.889	0.012	.
1	A	214	VAL	HG21	0.892	0.012	.
1	A	214	VAL	HG22	0.892	0.012	.
1	A	214	VAL	HG23	0.892	0.012	.
1	A	214	VAL	CG1	21.427	0.005	.
1	A	214	VAL	CG2	20.538	0.029	.
1	A	214	VAL	C	176.201	0.000	.
1	A	215	LYS	N	125.722	0.012	.
1	A	215	LYS	H	8.423	0.008	.
1	A	215	LYS	CA	56.348	0.034	.
1	A	215	LYS	HA	4.273	0.004	.
1	A	215	LYS	CB	32.987	0.016	.
1	A	215	LYS	HB2	1.804	0.007	.
1	A	215	LYS	HB3	1.746	0.010	.
1	A	215	LYS	CG	24.824	0.048	.
1	A	215	LYS	HG2	1.422	0.010	.
1	A	215	LYS	HG3	1.422	0.010	.
1	A	215	LYS	CD	28.952	0.073	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	215	LYS	HD2	1.667	0.011	.
1	A	215	LYS	HD3	1.667	0.011	.
1	A	215	LYS	CE	41.841	0.032	.
1	A	215	LYS	HE2	2.974	0.006	.
1	A	215	LYS	HE3	2.974	0.006	.
1	A	215	LYS	C	176.246	0.000	.
1	A	216	ALA	N	125.502	0.012	.
1	A	216	ALA	H	8.381	0.004	.
1	A	216	ALA	CA	52.59	0.021	.
1	A	216	ALA	HA	4.262	0.004	.
1	A	216	ALA	HB1	1.353	0.009	.
1	A	216	ALA	HB2	1.353	0.009	.
1	A	216	ALA	HB3	1.353	0.009	.
1	A	216	ALA	CB	19.407	0.000	.
1	A	216	ALA	C	177.369	0.000	.
1	A	217	ASP	N	119.376	0.030	.
1	A	217	ASP	H	8.284	0.002	.
1	A	217	ASP	CA	54.265	0.034	.
1	A	217	ASP	HA	4.555	0.005	.
1	A	217	ASP	CB	40.999	0.027	.
1	A	217	ASP	HB2	2.617	0.008	.
1	A	217	ASP	HB3	2.704	0.005	.
1	A	217	ASP	C	176.367	0.000	.
1	A	218	LEU	N	121.78	0.045	.
1	A	218	LEU	H	8.086	0.004	.
1	A	218	LEU	CA	55.335	0.004	.
1	A	218	LEU	HA	4.249	0.006	.
1	A	218	LEU	CB	42.262	0.003	.
1	A	218	LEU	HB2	1.525	0.003	.
1	A	218	LEU	HB3	1.601	0.005	.
1	A	218	LEU	CG	27.102	0.021	.
1	A	218	LEU	HG	1.599	0.011	.
1	A	218	LEU	HD11	0.882	0.011	.
1	A	218	LEU	HD12	0.882	0.011	.
1	A	218	LEU	HD13	0.882	0.011	.
1	A	218	LEU	HD21	0.824	0.004	.
1	A	218	LEU	HD22	0.824	0.004	.
1	A	218	LEU	HD23	0.824	0.004	.
1	A	218	LEU	CD1	25.233	0.008	.
1	A	218	LEU	CD2	23.605	0.036	.
1	A	218	LEU	C	177.535	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	219	GLU	N	120.262	0.060	.
1	A	219	GLU	H	8.218	0.002	.
1	A	219	GLU	CA	56.689	0.005	.
1	A	219	GLU	HA	4.128	0.010	.
1	A	219	GLU	CB	30.146	0.010	.
1	A	219	GLU	HB2	1.857	0.008	.
1	A	219	GLU	HB3	1.857	0.008	.
1	A	219	GLU	CG	36.276	0.009	.
1	A	219	GLU	HG2	2.176	0.001	.
1	A	219	GLU	HG3	2.095	0.008	.
1	A	219	GLU	C	176.266	0.000	.
1	A	220	HIS	N	119.284	0.025	.
1	A	220	HIS	H	8.148	0.005	.
1	A	220	HIS	CA	55.977	0.000	.
1	A	220	HIS	HA	4.53	0.011	.
1	A	220	HIS	CB	30.395	0.009	.
1	A	220	HIS	HB2	3.019	0.007	.
1	A	220	HIS	HB3	2.956	0.002	.
1	A	220	HIS	CD2	119.615	0.000	.
1	A	220	HIS	HD2	0.264	0.000	.
1	A	221	HIS	N	125.487	0.013	.
1	A	221	HIS	H	8.025	0.001	.
1	A	221	HIS	CA	57.407	0.000	.
1	A	221	HIS	HA	4.77	0.000	.
1	A	221	HIS	CB	46.978	0.000	.
1	A	221	HIS	HB2	3.01	0.000	.
1	A	221	HIS	HB3	3.01	0.000	.
1	A	221	HIS	CD2	119.959	0.000	.
1	A	221	HIS	HD2	7.0	0.000	.
1	A	222	HIS	N	126.0	0.000	.
1	A	222	HIS	H	8.012	0.000	.
1	A	222	HIS	CA	57.29	0.016	.
1	A	222	HIS	HA	4.387	0.001	.
1	A	222	HIS	CB	30.518	0.003	.
1	A	222	HIS	HB2	3.16	0.003	.
1	A	222	HIS	HB3	3.015	0.001	.

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	191	-0.05 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	173	-0.20 ± 0.23	None needed (< 0.5 ppm)
$^{13}\text{C}'$	181	0.26 ± 0.19	None needed (< 0.5 ppm)
^{15}N	171	-0.78 ± 0.51	None needed (imprecise)

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 93%, i.e. 1092 atoms were assigned a chemical shift out of a possible 1170. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	432/436 (99%)	177/179 (99%)	173/174 (99%)	82/83 (99%)
Sidechain	632/696 (91%)	427/454 (94%)	199/214 (93%)	6/28 (21%)
Aromatic	28/38 (74%)	16/19 (84%)	11/17 (65%)	1/2 (50%)
Overall	1092/1170 (93%)	620/652 (95%)	383/405 (95%)	89/113 (79%)

7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	220	HIS	HD2	0.26	4.65 – 9.35	-14.3
1	A	221	HIS	CB	46.98	19.76 – 40.75	8.0
1	A	136	GLY	N	132.75	91.59 – 127.52	6.5
1	A	128	LEU	HB3	-0.70	-0.26 – 3.31	-6.2
1	A	179	LYS	HD2	2.78	0.58 – 2.64	5.7
1	A	179	LYS	HD3	2.78	0.54 – 2.65	5.6
1	A	212	ARG	CG	20.79	21.24 – 33.19	-5.4
1	A	142	LYS	HG3	-0.04	0.04 – 2.67	-5.3

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

