



wwPDB NMR Structure Validation Summary Report ⓘ

Jun 22, 2024 – 08:21 PM EDT

PDB ID : 6CZT
BMRB ID : 30450
Title : CS-rosetta determined structures of the N-terminal domain of AlgF from P. aeruginosa
Authors : Tammam, S.; Howell, P.L.
Deposited on : 2018-04-09

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

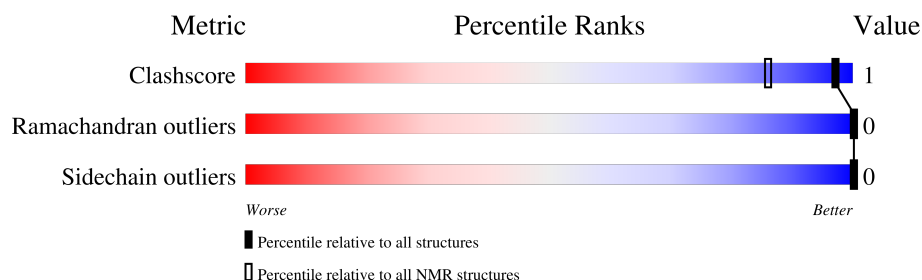
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 94%.

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	<div> <div style="width: 41%; background-color: green;"></div> <div style="width: 58%; background-color: grey;"></div> <div style="width: 1%; background-color: cyan;"></div> </div>

2 Ensemble composition and analysis

This entry contains 10 models. Model 3 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:40-A:119 (80)	1.71	3

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 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1185 atoms, of which 584 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms					Trace
1	A	82	Total	C	H	N	O	0
			1185	380	584	98	123	

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

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	954
Number of unparsed shifts	0
Number of shifts with mapping errors	1368
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

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	587	571	571	1±1
All	All	5870	5710	5710	7

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:105:LEU:C	1:A:105:LEU:HD23	0.47	2.30	9	1
1:A:43:SER:O	1:A:100:ASP:N	0.44	2.51	9	1
1:A:79:LEU:N	1:A:80:PRO:CD	0.44	2.81	9	3
1:A:56:LEU:HD12	1:A:56:LEU:C	0.43	2.33	4	1
1:A:79:LEU:N	1:A:80:PRO:HD2	0.42	2.28	2	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	79/196 (40%)	77±1 (98±2%)	2±1 (2±2%)	0±0 (0±0%)	100	100
All	All	790/1960 (40%)	773 (98%)	17 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	66/163 (40%)	66±0 (100±0%)	0±0 (0±0%)	100	100
All	All	660/1630 (40%)	660 (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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 94% for the well-defined parts and 94% 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

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	954
Number of unparsed shifts	0
Number of shifts with mapping errors	1368
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 1368) 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	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	.
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	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
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	.
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	124	LYS	N	121.249	0.043	.
1	A	124	LYS	H	8.287	0.010	.
1	A	124	LYS	CA	56.647	0.004	.
1	A	124	LYS	HA	4.018	0.007	.
1	A	124	LYS	CB	32.653	0.068	.
1	A	124	LYS	HB2	1.835	0.006	.
1	A	124	LYS	HB3	1.89	0.008	.
1	A	124	LYS	CG	25.064	0.058	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	124	LYS	HG2	1.276	0.008	.
1	A	124	LYS	HG3	1.337	0.009	.
1	A	124	LYS	CD	28.712	0.013	.
1	A	124	LYS	HD2	1.545	0.005	.
1	A	124	LYS	HD3	1.545	0.005	.
1	A	124	LYS	CE	41.845	0.025	.
1	A	124	LYS	HE2	2.88	0.012	.
1	A	124	LYS	HE3	2.88	0.012	.
1	A	124	LYS	C	176.526	0.000	.
1	A	125	GLN	N	114.943	0.011	.
1	A	125	GLN	H	8.269	0.002	.
1	A	125	GLN	CA	56.305	0.024	.
1	A	125	GLN	HA	4.394	0.008	.
1	A	125	GLN	CB	30.457	0.049	.
1	A	125	GLN	HB2	2.212	0.008	.
1	A	125	GLN	HB3	1.983	0.007	.
1	A	125	GLN	CG	33.854	0.041	.
1	A	125	GLN	HG2	2.345	0.008	.
1	A	125	GLN	HG3	2.271	0.010	.
1	A	125	GLN	CD	180.107	0.000	.
1	A	125	GLN	NE2	112.147	0.021	.
1	A	125	GLN	HE21	6.816	0.009	.
1	A	125	GLN	HE22	7.497	0.006	.
1	A	125	GLN	C	175.903	0.000	.
1	A	126	LYS	N	117.842	0.024	.
1	A	126	LYS	H	7.334	0.007	.
1	A	126	LYS	CA	53.786	0.060	.
1	A	126	LYS	HA	4.586	0.007	.
1	A	126	LYS	CB	35.759	0.042	.
1	A	126	LYS	HB2	2.165	0.006	.
1	A	126	LYS	HB3	1.573	0.012	.
1	A	126	LYS	CG	25.366	0.055	.
1	A	126	LYS	HG2	1.54	0.012	.
1	A	126	LYS	HG3	1.258	0.005	.
1	A	126	LYS	CD	28.719	0.094	.
1	A	126	LYS	HD2	1.444	0.005	.
1	A	126	LYS	HD3	1.444	0.005	.
1	A	126	LYS	CE	42.029	0.000	.
1	A	126	LYS	HE2	2.893	0.004	.
1	A	126	LYS	HE3	2.893	0.004	.
1	A	126	LYS	C	174.078	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	127	ALA	N	122.728	0.025	.
1	A	127	ALA	H	8.746	0.009	.
1	A	127	ALA	CA	50.654	0.032	.
1	A	127	ALA	HA	4.952	0.011	.
1	A	127	ALA	HB1	1.21	0.010	.
1	A	127	ALA	HB2	1.21	0.010	.
1	A	127	ALA	HB3	1.21	0.010	.
1	A	127	ALA	CB	23.92	0.071	.
1	A	127	ALA	C	174.689	0.000	.
1	A	128	LEU	N	121.23	0.031	.
1	A	128	LEU	H	8.208	0.006	.
1	A	128	LEU	CA	53.485	0.000	.
1	A	128	LEU	HA	4.634	0.014	.
1	A	128	LEU	CB	44.625	0.016	.
1	A	128	LEU	HB2	0.963	0.011	.
1	A	128	LEU	HB3	-0.699	0.008	.
1	A	128	LEU	CG	25.95	0.073	.
1	A	128	LEU	HG	0.447	0.010	.
1	A	128	LEU	HD11	0.828	0.011	.
1	A	128	LEU	HD12	0.828	0.011	.
1	A	128	LEU	HD13	0.828	0.011	.
1	A	128	LEU	HD21	0.518	0.009	.
1	A	128	LEU	HD22	0.518	0.009	.
1	A	128	LEU	HD23	0.518	0.009	.
1	A	128	LEU	CD1	22.547	0.069	.
1	A	128	LEU	CD2	24.312	0.056	.
1	A	128	LEU	C	175.094	0.000	.
1	A	129	VAL	N	124.872	0.030	.
1	A	129	VAL	H	8.295	0.005	.
1	A	129	VAL	CA	59.797	0.042	.
1	A	129	VAL	HA	4.804	0.009	.
1	A	129	VAL	CB	33.513	0.047	.
1	A	129	VAL	HB	1.745	0.011	.
1	A	129	VAL	HG11	0.783	0.009	.
1	A	129	VAL	HG12	0.783	0.009	.
1	A	129	VAL	HG13	0.783	0.009	.
1	A	129	VAL	HG21	0.837	0.010	.
1	A	129	VAL	HG22	0.837	0.010	.
1	A	129	VAL	HG23	0.837	0.010	.
1	A	129	VAL	CG1	22.347	0.006	.
1	A	129	VAL	CG2	22.478	0.049	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	129	VAL	C	172.668	0.000	.
1	A	130	ARG	N	128.132	0.028	.
1	A	130	ARG	H	8.49	0.007	.
1	A	130	ARG	CA	52.798	0.040	.
1	A	130	ARG	HA	5.485	0.008	.
1	A	130	ARG	CB	33.956	0.033	.
1	A	130	ARG	HB2	1.78	0.009	.
1	A	130	ARG	HB3	1.558	0.011	.
1	A	130	ARG	CG	26.679	0.037	.
1	A	130	ARG	HG2	1.097	0.015	.
1	A	130	ARG	HG3	1.8	0.013	.
1	A	130	ARG	CD	43.12	0.024	.
1	A	130	ARG	HD2	2.986	0.013	.
1	A	130	ARG	HD3	3.092	0.009	.
1	A	130	ARG	NE	85.963	0.060	.
1	A	130	ARG	HE	9.642	0.006	.
1	A	130	ARG	C	175.553	0.000	.
1	A	131	VAL	N	126.448	0.016	.
1	A	131	VAL	H	9.406	0.007	.
1	A	131	VAL	CA	61.002	0.055	.
1	A	131	VAL	HA	4.478	0.007	.
1	A	131	VAL	CB	33.649	0.023	.
1	A	131	VAL	HB	1.987	0.007	.
1	A	131	VAL	HG11	0.819	0.011	.
1	A	131	VAL	HG12	0.819	0.011	.
1	A	131	VAL	HG13	0.819	0.011	.
1	A	131	VAL	HG21	0.691	0.013	.
1	A	131	VAL	HG22	0.691	0.013	.
1	A	131	VAL	HG23	0.691	0.013	.
1	A	131	VAL	CG1	22.513	0.054	.
1	A	131	VAL	CG2	20.141	0.049	.
1	A	131	VAL	C	175.552	0.000	.
1	A	132	GLN	N	127.553	0.053	.
1	A	132	GLN	H	8.666	0.004	.
1	A	132	GLN	CA	54.797	0.039	.
1	A	132	GLN	HA	4.549	0.009	.
1	A	132	GLN	CB	27.048	0.000	.
1	A	132	GLN	HB2	1.77	0.000	.
1	A	132	GLN	CG	30.71	0.000	.
1	A	132	GLN	HG2	2.993	0.000	.
1	A	132	GLN	NE2	107.994	0.054	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	132	GLN	HE21	6.993	0.006	.
1	A	132	GLN	HE22	5.857	0.013	.
1	A	132	GLN	C	173.309	0.000	.
1	A	133	ASN	N	119.558	0.039	.
1	A	133	ASN	H	8.345	0.005	.
1	A	133	ASN	CA	51.812	0.024	.
1	A	133	ASN	HA	4.687	0.012	.
1	A	133	ASN	CB	38.625	0.051	.
1	A	133	ASN	HB2	3.505	0.009	.
1	A	133	ASN	HB3	1.961	0.013	.
1	A	133	ASN	CG	176.104	0.000	.
1	A	133	ASN	ND2	113.593	0.059	.
1	A	133	ASN	HD21	6.509	0.007	.
1	A	133	ASN	HD22	7.94	0.006	.
1	A	133	ASN	C	173.931	0.000	.
1	A	134	LEU	N	127.534	0.028	.
1	A	134	LEU	H	8.723	0.007	.
1	A	134	LEU	CA	54.396	0.054	.
1	A	134	LEU	HA	4.682	0.008	.
1	A	134	LEU	CB	40.775	0.025	.
1	A	134	LEU	HB2	2.106	0.012	.
1	A	134	LEU	HB3	1.751	0.008	.
1	A	134	LEU	CG	28.893	0.019	.
1	A	134	LEU	HG	1.75	0.003	.
1	A	134	LEU	HD11	0.966	0.007	.
1	A	134	LEU	HD12	0.966	0.007	.
1	A	134	LEU	HD13	0.966	0.007	.
1	A	134	LEU	HD21	0.88	0.010	.
1	A	134	LEU	HD22	0.88	0.010	.
1	A	134	LEU	HD23	0.88	0.010	.
1	A	134	LEU	CD1	25.836	0.046	.
1	A	134	LEU	CD2	24.75	0.050	.
1	A	134	LEU	C	176.833	0.000	.
1	A	135	SER	N	120.492	0.030	.
1	A	135	SER	H	8.227	0.005	.
1	A	135	SER	CA	58.06	0.067	.
1	A	135	SER	HA	4.826	0.009	.
1	A	135	SER	CB	66.357	0.038	.
1	A	135	SER	HB2	4.04	0.007	.
1	A	135	SER	HB3	3.375	0.012	.
1	A	135	SER	C	172.659	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	136	GLY	N	132.747	0.021	.
1	A	136	GLY	H	7.989	0.007	.
1	A	136	GLY	CA	45.201	0.035	.
1	A	136	GLY	HA2	3.694	0.009	.
1	A	136	GLY	HA3	4.379	0.012	.
1	A	136	GLY	C	175.333	0.000	.
1	A	137	SER	N	118.625	0.023	.
1	A	137	SER	H	8.379	0.008	.
1	A	137	SER	CA	57.925	0.000	.
1	A	137	SER	HA	4.632	0.005	.
1	A	137	SER	CB	65.177	0.022	.
1	A	137	SER	HB2	3.387	0.010	.
1	A	137	SER	HB3	3.69	0.013	.
1	A	137	SER	C	171.342	0.000	.
1	A	138	LYS	N	124.644	0.032	.
1	A	138	LYS	H	8.695	0.004	.
1	A	138	LYS	CA	55.744	0.029	.
1	A	138	LYS	HA	4.573	0.007	.
1	A	138	LYS	CB	32.347	0.046	.
1	A	138	LYS	HB2	1.536	0.009	.
1	A	138	LYS	HB3	1.742	0.011	.
1	A	138	LYS	CG	24.528	0.049	.
1	A	138	LYS	HG2	1.06	0.006	.
1	A	138	LYS	HG3	0.95	0.011	.
1	A	138	LYS	CE	40.995	0.022	.
1	A	138	LYS	HE2	2.838	0.006	.
1	A	138	LYS	HE3	2.838	0.006	.
1	A	138	LYS	C	176.268	0.000	.
1	A	139	LEU	N	125.493	0.020	.
1	A	139	LEU	H	7.905	0.006	.
1	A	139	LEU	CA	53.902	0.011	.
1	A	139	LEU	HA	5.193	0.008	.
1	A	139	LEU	CB	46.978	0.000	.
1	A	139	LEU	HB2	1.308	0.010	.
1	A	139	LEU	HB3	1.307	0.010	.
1	A	139	LEU	CG	27.263	0.000	.
1	A	139	LEU	HG	1.43	0.000	.
1	A	139	LEU	HD11	0.662	0.008	.
1	A	139	LEU	HD12	0.662	0.008	.
1	A	139	LEU	HD13	0.662	0.008	.
1	A	139	LEU	HD21	0.671	0.007	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	139	LEU	HD22	0.671	0.007	.
1	A	139	LEU	HD23	0.671	0.007	.
1	A	139	LEU	CD1	27.137	0.054	.
1	A	139	LEU	CD2	22.838	0.058	.
1	A	139	LEU	C	175.514	0.000	.
1	A	140	THR	N	116.367	0.022	.
1	A	140	THR	H	9.031	0.008	.
1	A	140	THR	CA	61.319	0.054	.
1	A	140	THR	HA	4.949	0.013	.
1	A	140	THR	CB	73.289	0.061	.
1	A	140	THR	HB	3.933	0.009	.
1	A	140	THR	HG21	1.145	0.006	.
1	A	140	THR	HG22	1.145	0.006	.
1	A	140	THR	HG23	1.145	0.006	.
1	A	140	THR	CG2	22.499	0.050	.
1	A	140	THR	C	172.174	0.000	.
1	A	141	LEU	N	129.855	0.025	.
1	A	141	LEU	H	9.56	0.005	.
1	A	141	LEU	CA	53.335	0.035	.
1	A	141	LEU	HA	5.14	0.013	.
1	A	141	LEU	CB	45.864	0.032	.
1	A	141	LEU	HB2	1.943	0.011	.
1	A	141	LEU	HB3	1.087	0.008	.
1	A	141	LEU	CG	26.979	0.016	.
1	A	141	LEU	HG	1.409	0.011	.
1	A	141	LEU	HD11	0.805	0.007	.
1	A	141	LEU	HD12	0.805	0.007	.
1	A	141	LEU	HD13	0.805	0.007	.
1	A	141	LEU	HD21	0.809	0.011	.
1	A	141	LEU	HD22	0.809	0.011	.
1	A	141	LEU	HD23	0.809	0.011	.
1	A	141	LEU	CD1	25.568	0.050	.
1	A	141	LEU	CD2	23.728	0.070	.
1	A	141	LEU	C	174.796	0.000	.
1	A	142	LYS	N	126.478	0.030	.
1	A	142	LYS	H	9.156	0.005	.
1	A	142	LYS	CA	55.164	0.026	.
1	A	142	LYS	HA	5.372	0.011	.
1	A	142	LYS	CB	37.64	0.029	.
1	A	142	LYS	HB2	1.616	0.008	.
1	A	142	LYS	HB3	1.675	0.010	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	142	LYS	CG	28.742	0.037	.
1	A	142	LYS	HG2	0.58	0.007	.
1	A	142	LYS	HG3	-0.036	0.006	.
1	A	142	LYS	CD	27.322	0.033	.
1	A	142	LYS	HD2	1.455	0.013	.
1	A	142	LYS	HD3	1.455	0.013	.
1	A	142	LYS	CE	41.522	0.009	.
1	A	142	LYS	HE2	2.124	0.005	.
1	A	142	LYS	HE3	2.124	0.005	.
1	A	142	LYS	C	176.512	0.000	.
1	A	143	THR	N	109.413	0.051	.
1	A	143	THR	H	8.34	0.007	.
1	A	143	THR	CA	63.417	0.041	.
1	A	143	THR	HA	4.44	0.010	.
1	A	143	THR	CB	69.119	0.043	.
1	A	143	THR	HB	4.724	0.013	.
1	A	143	THR	HG21	1.189	0.011	.
1	A	143	THR	HG22	1.189	0.011	.
1	A	143	THR	HG23	1.189	0.011	.
1	A	143	THR	CG2	23.799	0.035	.
1	A	143	THR	C	176.984	0.000	.
1	A	144	ALA	N	123.679	0.040	.
1	A	144	ALA	H	8.263	0.005	.
1	A	144	ALA	CA	55.406	0.027	.
1	A	144	ALA	HA	3.956	0.007	.
1	A	144	ALA	HB1	1.298	0.008	.
1	A	144	ALA	HB2	1.298	0.008	.
1	A	144	ALA	HB3	1.298	0.008	.
1	A	144	ALA	CB	18.048	0.056	.
1	A	144	ALA	C	177.61	0.000	.
1	A	145	ASP	N	113.872	0.049	.
1	A	145	ASP	H	7.848	0.010	.
1	A	145	ASP	CA	53.57	0.056	.
1	A	145	ASP	HA	4.395	0.011	.
1	A	145	ASP	CB	40.083	0.012	.
1	A	145	ASP	HB2	2.999	0.008	.
1	A	145	ASP	HB3	2.689	0.006	.
1	A	145	ASP	C	177.437	0.000	.
1	A	146	GLY	N	108.862	0.021	.
1	A	146	GLY	H	8.674	0.002	.
1	A	146	GLY	CA	45.723	0.016	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	146	GLY	HA2	4.012	0.008	.
1	A	146	GLY	HA3	3.244	0.009	.
1	A	146	GLY	C	174.727	0.000	.
1	A	147	LYS	N	118.33	0.035	.
1	A	147	LYS	H	8.1	0.003	.
1	A	147	LYS	CA	58.261	0.056	.
1	A	147	LYS	HA	4.013	0.004	.
1	A	147	LYS	CB	33.286	0.018	.
1	A	147	LYS	HB2	1.708	0.010	.
1	A	147	LYS	HB3	1.705	0.013	.
1	A	147	LYS	CG	28.767	0.060	.
1	A	147	LYS	HG2	1.543	0.009	.
1	A	147	LYS	HG3	1.541	0.008	.
1	A	147	LYS	CD	25.319	0.045	.
1	A	147	LYS	HD2	1.22	0.014	.
1	A	147	LYS	HD3	1.176	0.003	.
1	A	147	LYS	CE	41.836	0.040	.
1	A	147	LYS	HE2	2.893	0.007	.
1	A	147	LYS	HE3	2.893	0.007	.
1	A	147	LYS	C	176.982	0.000	.
1	A	148	THR	N	113.507	0.009	.
1	A	148	THR	H	7.219	0.007	.
1	A	148	THR	CA	61.641	0.041	.
1	A	148	THR	HA	4.424	0.007	.
1	A	148	THR	CB	70.372	0.035	.
1	A	148	THR	HB	4.108	0.003	.
1	A	148	THR	HG21	1.073	0.007	.
1	A	148	THR	HG22	1.073	0.007	.
1	A	148	THR	HG23	1.073	0.007	.
1	A	148	THR	CG2	21.443	0.054	.
1	A	148	THR	C	177.765	0.000	.
1	A	149	ASP	N	126.176	0.030	.
1	A	149	ASP	H	8.746	0.008	.
1	A	149	ASP	CA	55.229	0.024	.
1	A	149	ASP	HA	4.479	0.007	.
1	A	149	ASP	CB	41.36	0.043	.
1	A	149	ASP	HB2	2.476	0.011	.
1	A	149	ASP	HB3	2.034	0.010	.
1	A	149	ASP	C	175.173	0.000	.
1	A	150	VAL	N	124.478	0.027	.
1	A	150	VAL	H	9.0	0.004	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	150	VAL	CA	64.574	0.026	.
1	A	150	VAL	HA	3.945	0.010	.
1	A	150	VAL	CB	32.638	0.061	.
1	A	150	VAL	HB	1.609	0.008	.
1	A	150	VAL	CG1	21.318	0.048	.
1	A	150	VAL	CG2	21.31	0.048	.
1	A	150	VAL	HG11	0.809	0.009	.
1	A	150	VAL	HG12	0.809	0.009	.
1	A	150	VAL	HG13	0.809	0.009	.
1	A	150	VAL	HG21	0.809	0.009	.
1	A	150	VAL	HG22	0.809	0.009	.
1	A	150	VAL	HG23	0.809	0.009	.
1	A	150	VAL	C	175.549	0.000	.
1	A	151	VAL	N	115.605	0.016	.
1	A	151	VAL	H	7.62	0.003	.
1	A	151	VAL	CA	61.821	0.016	.
1	A	151	VAL	HA	4.216	0.008	.
1	A	151	VAL	CB	34.652	0.017	.
1	A	151	VAL	HB	1.782	0.007	.
1	A	151	VAL	HG11	0.751	0.011	.
1	A	151	VAL	HG12	0.751	0.011	.
1	A	151	VAL	HG13	0.751	0.011	.
1	A	151	VAL	HG21	0.749	0.011	.
1	A	151	VAL	HG22	0.749	0.011	.
1	A	151	VAL	HG23	0.749	0.011	.
1	A	151	VAL	CG1	22.069	0.040	.
1	A	151	VAL	CG2	21.566	0.055	.
1	A	151	VAL	C	174.098	0.000	.
1	A	152	LYS	N	128.009	0.014	.
1	A	152	LYS	H	8.978	0.006	.
1	A	152	LYS	CA	55.739	0.040	.
1	A	152	LYS	HA	4.552	0.008	.
1	A	152	LYS	CB	35.803	0.007	.
1	A	152	LYS	HB2	1.715	0.008	.
1	A	152	LYS	HB3	1.455	0.007	.
1	A	152	LYS	CG	25.035	0.047	.
1	A	152	LYS	HG2	1.222	0.006	.
1	A	152	LYS	HG3	1.181	0.008	.
1	A	152	LYS	CD	29.217	0.040	.
1	A	152	LYS	HD2	1.538	0.007	.
1	A	152	LYS	HD3	1.538	0.007	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	152	LYS	CE	41.787	0.034	.
1	A	152	LYS	HE2	2.888	0.008	.
1	A	152	LYS	HE3	2.888	0.008	.
1	A	152	LYS	C	174.824	0.000	.
1	A	153	ASP	N	122.843	0.008	.
1	A	153	ASP	H	8.355	0.008	.
1	A	153	ASP	CA	55.45	0.019	.
1	A	153	ASP	HA	3.74	0.007	.
1	A	153	ASP	CB	39.387	0.039	.
1	A	153	ASP	HB2	2.595	0.007	.
1	A	153	ASP	HB3	2.519	0.004	.
1	A	153	ASP	C	174.212	0.000	.
1	A	154	VAL	N	121.232	0.024	.
1	A	154	VAL	H	9.296	0.003	.
1	A	154	VAL	CA	62.068	0.001	.
1	A	154	VAL	HA	3.874	0.008	.
1	A	154	VAL	CB	31.084	0.072	.
1	A	154	VAL	HB	1.899	0.014	.
1	A	154	VAL	HG11	0.771	0.011	.
1	A	154	VAL	HG12	0.771	0.011	.
1	A	154	VAL	HG13	0.771	0.011	.
1	A	154	VAL	HG21	0.718	0.009	.
1	A	154	VAL	HG22	0.718	0.009	.
1	A	154	VAL	HG23	0.718	0.009	.
1	A	154	VAL	CG1	22.641	0.026	.
1	A	154	VAL	CG2	22.269	0.040	.
1	A	154	VAL	C	177.189	0.000	.
1	A	155	GLY	N	117.42	0.029	.
1	A	155	GLY	H	8.756	0.010	.
1	A	155	GLY	CA	44.76	0.022	.
1	A	155	GLY	HA2	3.793	0.010	.
1	A	155	GLY	HA3	3.946	0.009	.
1	A	155	GLY	C	177.189	0.000	.
1	A	156	PRO	CD	50.094	0.041	.
1	A	156	PRO	CA	63.807	0.052	.
1	A	156	PRO	HA	4.051	0.007	.
1	A	156	PRO	CB	33.034	0.026	.
1	A	156	PRO	HB2	2.425	0.007	.
1	A	156	PRO	HB3	1.802	0.007	.
1	A	156	PRO	CG	27.487	0.039	.
1	A	156	PRO	HG2	1.922	0.009	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	156	PRO	HG3	1.579	0.009	.
1	A	156	PRO	HD2	3.457	0.007	.
1	A	156	PRO	HD3	3.147	0.009	.
1	A	156	PRO	C	177.632	0.000	.
1	A	157	GLN	N	118.922	0.035	.
1	A	157	GLN	H	8.109	0.008	.
1	A	157	GLN	CA	56.082	0.005	.
1	A	157	GLN	HA	4.056	0.004	.
1	A	157	GLN	CB	25.445	0.002	.
1	A	157	GLN	HB2	2.209	0.008	.
1	A	157	GLN	HB3	2.323	0.008	.
1	A	157	GLN	CG	33.462	0.050	.
1	A	157	GLN	HG2	2.416	0.007	.
1	A	157	GLN	HG3	2.28	0.013	.
1	A	157	GLN	CD	180.544	0.000	.
1	A	157	GLN	NE2	111.753	0.029	.
1	A	157	GLN	HE21	7.369	0.008	.
1	A	157	GLN	HE22	6.798	0.002	.
1	A	157	GLN	C	174.807	0.000	.
1	A	158	SER	N	112.567	0.012	.
1	A	158	SER	H	7.882	0.003	.
1	A	158	SER	CA	56.833	0.034	.
1	A	158	SER	HA	4.95	0.012	.
1	A	158	SER	CB	65.196	0.027	.
1	A	158	SER	HB2	3.73	0.009	.
1	A	158	SER	HB3	3.781	0.011	.
1	A	158	SER	C	172.202	0.000	.
1	A	159	HIS	N	116.376	0.027	.
1	A	159	HIS	H	8.109	0.005	.
1	A	159	HIS	CA	54.084	0.008	.
1	A	159	HIS	HA	6.011	0.011	.
1	A	159	HIS	CB	33.434	0.040	.
1	A	159	HIS	HB2	2.826	0.015	.
1	A	159	HIS	HB3	3.01	0.014	.
1	A	159	HIS	CD2	120.695	0.057	.
1	A	159	HIS	HD2	6.929	0.017	.
1	A	160	GLY	N	106.528	0.018	.
1	A	160	GLY	H	8.099	0.005	.
1	A	160	GLY	CA	45.61	0.046	.
1	A	160	GLY	HA2	4.247	0.010	.
1	A	160	GLY	HA3	3.508	0.011	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	160	GLY	C	170.847	0.000	.
1	A	161	ASP	N	122.191	0.037	.
1	A	161	ASP	H	8.471	0.004	.
1	A	161	ASP	CA	53.349	0.025	.
1	A	161	ASP	HA	5.648	0.008	.
1	A	161	ASP	CB	45.255	0.013	.
1	A	161	ASP	HB2	2.519	0.012	.
1	A	161	ASP	HB3	2.582	0.008	.
1	A	161	ASP	C	176.417	0.000	.
1	A	162	ARG	N	119.735	0.035	.
1	A	162	ARG	H	8.751	0.009	.
1	A	162	ARG	CA	55.052	0.035	.
1	A	162	ARG	HA	4.426	0.010	.
1	A	162	ARG	CB	34.252	0.028	.
1	A	162	ARG	HB2	1.777	0.007	.
1	A	162	ARG	HB3	1.47	0.007	.
1	A	162	ARG	CG	26.801	0.028	.
1	A	162	ARG	HG2	1.535	0.013	.
1	A	162	ARG	HG3	1.646	0.008	.
1	A	162	ARG	CD	42.577	0.019	.
1	A	162	ARG	HD2	3.336	0.005	.
1	A	162	ARG	HD3	3.479	0.005	.
1	A	162	ARG	C	174.136	0.000	.
1	A	163	GLU	N	128.516	0.016	.
1	A	163	GLU	H	8.717	0.009	.
1	A	163	GLU	CA	55.999	0.010	.
1	A	163	GLU	HA	4.961	0.010	.
1	A	163	GLU	CB	30.912	0.047	.
1	A	163	GLU	HB2	2.003	0.006	.
1	A	163	GLU	HB3	1.87	0.006	.
1	A	163	GLU	CG	37.557	0.029	.
1	A	163	GLU	HG2	2.411	0.008	.
1	A	163	GLU	HG3	2.17	0.010	.
1	A	163	GLU	C	176.482	0.000	.
1	A	164	ILE	N	122.983	0.024	.
1	A	164	ILE	H	9.049	0.010	.
1	A	164	ILE	CA	59.578	0.000	.
1	A	164	ILE	HA	4.639	0.010	.
1	A	164	ILE	CB	43.196	0.012	.
1	A	164	ILE	HB	1.664	0.007	.
1	A	164	ILE	HG21	0.752	0.011	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	164	ILE	HG22	0.752	0.011	.
1	A	164	ILE	HG23	0.752	0.011	.
1	A	164	ILE	CG2	17.083	0.061	.
1	A	164	ILE	CG1	26.459	0.037	.
1	A	164	ILE	HG12	1.013	0.006	.
1	A	164	ILE	HG13	1.323	0.007	.
1	A	164	ILE	HD11	0.657	0.005	.
1	A	164	ILE	HD12	0.657	0.005	.
1	A	164	ILE	HD13	0.657	0.005	.
1	A	164	ILE	CD1	13.947	0.034	.
1	A	164	ILE	C	173.799	0.000	.
1	A	165	ASN	N	122.173	0.032	.
1	A	165	ASN	H	8.182	0.009	.
1	A	165	ASN	CA	52.031	0.021	.
1	A	165	ASN	HA	4.862	0.007	.
1	A	165	ASN	CB	37.175	0.034	.
1	A	165	ASN	HB2	2.622	0.011	.
1	A	165	ASN	HB3	2.741	0.010	.
1	A	165	ASN	CG	176.297	0.000	.
1	A	165	ASN	ND2	113.592	0.035	.
1	A	165	ASN	HD21	7.616	0.005	.
1	A	165	ASN	HD22	7.146	0.007	.
1	A	165	ASN	C	173.799	0.000	.
1	A	166	PRO	CD	50.276	0.037	.
1	A	166	PRO	CA	63.632	0.030	.
1	A	166	PRO	HA	4.089	0.010	.
1	A	166	PRO	CB	30.241	0.021	.
1	A	166	PRO	HB2	1.668	0.010	.
1	A	166	PRO	HB3	2.106	0.009	.
1	A	166	PRO	CG	28.238	0.049	.
1	A	166	PRO	HG2	2.11	0.009	.
1	A	166	PRO	HG3	2.11	0.009	.
1	A	166	PRO	HD2	3.703	0.008	.
1	A	166	PRO	HD3	3.703	0.008	.
1	A	166	PRO	C	174.527	0.000	.
1	A	167	VAL	N	120.539	0.037	.
1	A	167	VAL	H	7.507	0.003	.
1	A	167	VAL	CA	59.696	0.045	.
1	A	167	VAL	HA	4.455	0.005	.
1	A	167	VAL	CB	35.312	0.002	.
1	A	167	VAL	HB	2.223	0.010	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	167	VAL	HG11	0.734	0.011	.
1	A	167	VAL	HG12	0.734	0.011	.
1	A	167	VAL	HG13	0.734	0.011	.
1	A	167	VAL	HG21	0.757	0.007	.
1	A	167	VAL	HG22	0.757	0.007	.
1	A	167	VAL	HG23	0.757	0.007	.
1	A	167	VAL	CG1	21.34	0.074	.
1	A	167	VAL	CG2	18.818	0.066	.
1	A	167	VAL	C	173.756	0.000	.
1	A	168	LYS	N	121.958	0.009	.
1	A	168	LYS	H	7.883	0.002	.
1	A	168	LYS	CA	55.961	0.042	.
1	A	168	LYS	HA	4.968	0.009	.
1	A	168	LYS	CB	32.562	0.063	.
1	A	168	LYS	HB2	1.656	0.007	.
1	A	168	LYS	HB3	1.557	0.011	.
1	A	168	LYS	CG	24.633	0.015	.
1	A	168	LYS	HG2	1.027	0.007	.
1	A	168	LYS	HG3	1.101	0.007	.
1	A	168	LYS	CD	29.533	0.007	.
1	A	168	LYS	HD2	1.544	0.010	.
1	A	168	LYS	HD3	1.544	0.010	.
1	A	168	LYS	CE	41.964	0.000	.
1	A	168	LYS	C	176.408	0.000	.
1	A	169	VAL	N	121.851	0.041	.
1	A	169	VAL	H	8.752	0.005	.
1	A	169	VAL	CA	59.522	0.069	.
1	A	169	VAL	HA	4.657	0.006	.
1	A	169	VAL	CB	35.157	0.032	.
1	A	169	VAL	HB	1.817	0.007	.
1	A	169	VAL	HG11	0.751	0.009	.
1	A	169	VAL	HG12	0.751	0.009	.
1	A	169	VAL	HG13	0.751	0.009	.
1	A	169	VAL	HG21	0.78	0.008	.
1	A	169	VAL	HG22	0.78	0.008	.
1	A	169	VAL	HG23	0.78	0.008	.
1	A	169	VAL	CG1	21.5	0.056	.
1	A	169	VAL	CG2	19.941	0.039	.
1	A	169	VAL	C	173.72	0.000	.
1	A	170	ASN	N	124.542	0.034	.
1	A	170	ASN	H	8.591	0.004	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	170	ASN	CA	52.711	0.014	.
1	A	170	ASN	HA	5.056	0.009	.
1	A	170	ASN	CB	39.362	0.039	.
1	A	170	ASN	HB2	2.705	0.008	.
1	A	170	ASN	HB3	2.705	0.008	.
1	A	170	ASN	CG	176.787	0.000	.
1	A	170	ASN	ND2	111.685	0.040	.
1	A	170	ASN	HD21	7.529	0.004	.
1	A	170	ASN	HD22	6.746	0.004	.
1	A	170	ASN	C	173.845	0.000	.
1	A	171	LEU	N	125.029	0.034	.
1	A	171	LEU	H	9.118	0.006	.
1	A	171	LEU	CA	53.496	0.088	.
1	A	171	LEU	HA	5.119	0.013	.
1	A	171	LEU	CB	45.301	0.056	.
1	A	171	LEU	HB2	1.963	0.011	.
1	A	171	LEU	HB3	1.719	0.010	.
1	A	171	LEU	CG	27.457	0.033	.
1	A	171	LEU	HG	1.568	0.009	.
1	A	171	LEU	HD11	0.781	0.015	.
1	A	171	LEU	HD12	0.781	0.015	.
1	A	171	LEU	HD13	0.781	0.015	.
1	A	171	LEU	HD21	0.972	0.007	.
1	A	171	LEU	HD22	0.972	0.007	.
1	A	171	LEU	HD23	0.972	0.007	.
1	A	171	LEU	CD1	26.721	0.041	.
1	A	171	LEU	CD2	26.612	0.062	.
1	A	171	LEU	C	175.057	0.000	.
1	A	172	ALA	N	120.839	0.014	.
1	A	172	ALA	H	9.349	0.007	.
1	A	172	ALA	CA	51.782	0.018	.
1	A	172	ALA	HA	4.793	0.010	.
1	A	172	ALA	HB1	1.512	0.009	.
1	A	172	ALA	HB2	1.512	0.009	.
1	A	172	ALA	HB3	1.512	0.009	.
1	A	172	ALA	CB	24.257	0.064	.
1	A	172	ALA	C	174.246	0.000	.
1	A	173	LEU	N	121.462	0.024	.
1	A	173	LEU	H	8.48	0.006	.
1	A	173	LEU	CA	53.325	0.042	.
1	A	173	LEU	HA	5.092	0.011	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	173	LEU	CB	46.266	0.056	.
1	A	173	LEU	HB2	1.089	0.009	.
1	A	173	LEU	HB3	1.628	0.010	.
1	A	173	LEU	CG	26.464	0.020	.
1	A	173	LEU	HG	1.408	0.009	.
1	A	173	LEU	HD11	0.688	0.009	.
1	A	173	LEU	HD12	0.688	0.009	.
1	A	173	LEU	HD13	0.688	0.009	.
1	A	173	LEU	HD21	0.815	0.008	.
1	A	173	LEU	HD22	0.815	0.008	.
1	A	173	LEU	HD23	0.815	0.008	.
1	A	173	LEU	CD1	25.663	0.067	.
1	A	173	LEU	CD2	23.74	0.072	.
1	A	173	LEU	C	174.688	0.000	.
1	A	174	PHE	N	126.714	0.015	.
1	A	174	PHE	H	9.739	0.005	.
1	A	174	PHE	CA	57.058	0.043	.
1	A	174	PHE	HA	4.995	0.012	.
1	A	174	PHE	CB	42.739	0.016	.
1	A	174	PHE	HB2	3.041	0.007	.
1	A	174	PHE	HB3	2.833	0.010	.
1	A	174	PHE	HD1	6.932	0.010	.
1	A	174	PHE	HD2	6.932	0.010	.
1	A	174	PHE	HE1	7.189	0.008	.
1	A	174	PHE	HE2	7.189	0.008	.
1	A	174	PHE	CD1	131.415	0.076	.
1	A	174	PHE	CE1	129.565	0.000	.
1	A	174	PHE	CZ	125.034	0.000	.
1	A	174	PHE	HZ	6.908	0.009	.
1	A	174	PHE	C	173.591	0.000	.
1	A	175	ASP	N	121.534	0.037	.
1	A	175	ASP	H	8.874	0.004	.
1	A	175	ASP	CA	52.079	0.045	.
1	A	175	ASP	HA	4.932	0.008	.
1	A	175	ASP	CB	41.487	0.026	.
1	A	175	ASP	HB2	2.688	0.009	.
1	A	175	ASP	HB3	2.246	0.005	.
1	A	175	ASP	C	177.229	0.000	.
1	A	176	GLY	N	113.944	0.015	.
1	A	176	GLY	H	8.64	0.004	.
1	A	176	GLY	CA	46.941	0.038	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	176	GLY	HA2	4.08	0.004	.
1	A	176	GLY	HA3	3.652	0.006	.
1	A	176	GLY	C	177.229	0.000	.
1	A	177	SER	N	121.605	0.040	.
1	A	177	SER	H	8.987	0.011	.
1	A	177	SER	CA	58.462	0.001	.
1	A	177	SER	HA	4.487	0.007	.
1	A	177	SER	CB	63.744	0.018	.
1	A	177	SER	HB2	3.878	0.004	.
1	A	177	SER	HB3	4.01	0.005	.
1	A	177	SER	C	174.024	0.000	.
1	A	178	LYS	N	123.594	0.042	.
1	A	178	LYS	H	8.097	0.008	.
1	A	178	LYS	CA	55.026	0.028	.
1	A	178	LYS	HA	4.443	0.010	.
1	A	178	LYS	CB	34.065	0.035	.
1	A	178	LYS	HB2	1.886	0.009	.
1	A	178	LYS	HB3	1.815	0.007	.
1	A	178	LYS	CG	24.495	0.069	.
1	A	178	LYS	HG2	1.362	0.010	.
1	A	178	LYS	HG3	1.272	0.005	.
1	A	178	LYS	CD	28.971	0.015	.
1	A	178	LYS	HD2	1.636	0.006	.
1	A	178	LYS	HD3	1.636	0.006	.
1	A	178	LYS	CE	41.8	0.031	.
1	A	178	LYS	HE2	2.927	0.005	.
1	A	178	LYS	HE3	2.927	0.005	.
1	A	178	LYS	C	174.6	0.000	.
1	A	179	LYS	N	127.762	0.052	.
1	A	179	LYS	H	8.667	0.006	.
1	A	179	LYS	CA	57.595	0.000	.
1	A	179	LYS	CB	31.323	0.010	.
1	A	179	LYS	HB2	1.02	0.005	.
1	A	179	LYS	HB3	1.419	0.007	.
1	A	179	LYS	CG	25.162	0.010	.
1	A	179	LYS	HG2	0.415	0.008	.
1	A	179	LYS	HG3	0.722	0.008	.
1	A	179	LYS	CD	27.899	0.024	.
1	A	179	LYS	HD2	2.784	0.009	.
1	A	179	LYS	HD3	2.784	0.009	.
1	A	179	LYS	C	176.423	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	180	VAL	N	126.156	0.011	.
1	A	180	VAL	H	9.045	0.008	.
1	A	180	VAL	CA	62.843	0.009	.
1	A	180	VAL	HA	4.069	0.009	.
1	A	180	VAL	CB	33.037	0.031	.
1	A	180	VAL	HB	1.736	0.010	.
1	A	180	VAL	HG11	0.824	0.011	.
1	A	180	VAL	HG12	0.824	0.011	.
1	A	180	VAL	HG13	0.824	0.011	.
1	A	180	VAL	HG21	0.666	0.009	.
1	A	180	VAL	HG22	0.666	0.009	.
1	A	180	VAL	HG23	0.666	0.009	.
1	A	180	VAL	CG1	21.633	0.045	.
1	A	180	VAL	CG2	20.78	0.038	.
1	A	180	VAL	C	176.326	0.000	.
1	A	181	SER	N	110.074	0.019	.
1	A	181	SER	H	7.145	0.008	.
1	A	181	SER	CA	58.466	0.044	.
1	A	181	SER	HA	4.451	0.008	.
1	A	181	SER	CB	65.579	0.036	.
1	A	181	SER	HB2	3.699	0.008	.
1	A	181	SER	HB3	3.406	0.008	.
1	A	181	SER	C	174.088	0.000	.
1	A	182	ASP	N	126.451	0.036	.
1	A	182	ASP	H	8.739	0.005	.
1	A	182	ASP	CA	55.572	0.022	.
1	A	182	ASP	HA	4.865	0.011	.
1	A	182	ASP	CB	41.388	0.042	.
1	A	182	ASP	HB2	2.474	0.009	.
1	A	182	ASP	HB3	2.715	0.005	.
1	A	182	ASP	C	175.75	0.000	.
1	A	183	LEU	N	121.465	0.048	.
1	A	183	LEU	H	8.165	0.005	.
1	A	183	LEU	CA	53.329	0.017	.
1	A	183	LEU	HA	4.658	0.008	.
1	A	183	LEU	CB	42.999	0.032	.
1	A	183	LEU	HB2	1.883	0.008	.
1	A	183	LEU	HB3	1.511	0.009	.
1	A	183	LEU	CG	27.435	0.019	.
1	A	183	LEU	HG	1.395	0.013	.
1	A	183	LEU	HD11	0.515	0.009	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	183	LEU	HD12	0.515	0.009	.
1	A	183	LEU	HD13	0.515	0.009	.
1	A	183	LEU	HD21	0.557	0.009	.
1	A	183	LEU	HD22	0.557	0.009	.
1	A	183	LEU	HD23	0.557	0.009	.
1	A	183	LEU	CD1	27.872	0.037	.
1	A	183	LEU	CD2	23.553	0.042	.
1	A	183	LEU	C	177.003	0.000	.
1	A	184	LYS	N	122.957	0.041	.
1	A	184	LYS	H	8.891	0.002	.
1	A	184	LYS	CA	55.309	0.027	.
1	A	184	LYS	HA	4.539	0.005	.
1	A	184	LYS	CB	32.029	0.044	.
1	A	184	LYS	HB2	1.893	0.009	.
1	A	184	LYS	HB3	2.044	0.012	.
1	A	184	LYS	CG	29.126	0.040	.
1	A	184	LYS	HG2	1.866	0.010	.
1	A	184	LYS	HG3	1.864	0.009	.
1	A	184	LYS	CD	25.461	0.076	.
1	A	184	LYS	HD2	1.72	0.003	.
1	A	184	LYS	HD3	1.78	0.007	.
1	A	184	LYS	CE	41.997	0.028	.
1	A	184	LYS	HE2	3.11	0.009	.
1	A	184	LYS	HE3	3.11	0.009	.
1	A	184	LYS	C	177.003	0.000	.
1	A	185	PRO	CD	50.75	0.032	.
1	A	185	PRO	CA	63.348	0.030	.
1	A	185	PRO	HA	4.663	0.006	.
1	A	185	PRO	CB	32.208	0.041	.
1	A	185	PRO	HB2	2.208	0.009	.
1	A	185	PRO	HB3	1.668	0.009	.
1	A	185	PRO	CG	27.697	0.020	.
1	A	185	PRO	HG2	2.064	0.008	.
1	A	185	PRO	HG3	2.063	0.007	.
1	A	185	PRO	HD2	3.971	0.010	.
1	A	185	PRO	HD3	3.669	0.006	.
1	A	185	PRO	C	175.46	0.000	.
1	A	186	VAL	N	118.867	0.032	.
1	A	186	VAL	H	7.686	0.006	.
1	A	186	VAL	CA	59.317	0.028	.
1	A	186	VAL	HA	4.227	0.005	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	186	VAL	CB	35.18	0.001	.
1	A	186	VAL	HB	0.751	0.008	.
1	A	186	VAL	HG11	0.004	0.005	.
1	A	186	VAL	HG12	0.004	0.005	.
1	A	186	VAL	HG13	0.004	0.005	.
1	A	186	VAL	HG21	-0.271	0.005	.
1	A	186	VAL	HG22	-0.271	0.005	.
1	A	186	VAL	HG23	-0.271	0.005	.
1	A	186	VAL	CG1	20.593	0.056	.
1	A	186	VAL	CG2	19.21	0.054	.
1	A	186	VAL	C	172.439	0.000	.
1	A	187	THR	N	121.648	0.027	.
1	A	187	THR	H	8.465	0.004	.
1	A	187	THR	CA	61.943	0.032	.
1	A	187	THR	HA	4.329	0.013	.
1	A	187	THR	CB	68.814	0.069	.
1	A	187	THR	HB	3.798	0.003	.
1	A	187	THR	HG21	0.919	0.007	.
1	A	187	THR	HG22	0.919	0.007	.
1	A	187	THR	HG23	0.919	0.007	.
1	A	187	THR	CG2	21.709	0.060	.
1	A	187	THR	C	173.294	0.000	.
1	A	188	LEU	N	127.441	0.045	.
1	A	188	LEU	H	7.65	0.007	.
1	A	188	LEU	CA	54.132	0.018	.
1	A	188	LEU	HA	4.331	0.008	.
1	A	188	LEU	CB	43.049	0.054	.
1	A	188	LEU	HB2	1.535	0.013	.
1	A	188	LEU	HB3	1.234	0.013	.
1	A	188	LEU	CG	27.752	0.063	.
1	A	188	LEU	HG	1.418	0.009	.
1	A	188	LEU	HD11	0.652	0.008	.
1	A	188	LEU	HD12	0.652	0.008	.
1	A	188	LEU	HD13	0.652	0.008	.
1	A	188	LEU	HD21	0.489	0.007	.
1	A	188	LEU	HD22	0.489	0.007	.
1	A	188	LEU	HD23	0.489	0.007	.
1	A	188	LEU	CD1	26.729	0.054	.
1	A	188	LEU	CD2	25.546	0.052	.
1	A	188	LEU	C	174.47	0.000	.
1	A	189	ALA	N	124.328	0.026	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	189	ALA	H	8.553	0.006	.
1	A	189	ALA	CA	49.772	0.039	.
1	A	189	ALA	HA	4.489	0.008	.
1	A	189	ALA	HB1	1.254	0.008	.
1	A	189	ALA	HB2	1.254	0.008	.
1	A	189	ALA	HB3	1.254	0.008	.
1	A	189	ALA	CB	21.146	0.043	.
1	A	189	ALA	C	176.788	0.000	.
1	A	190	ARG	N	118.848	0.024	.
1	A	190	ARG	H	8.419	0.003	.
1	A	190	ARG	CA	58.189	0.004	.
1	A	190	ARG	HA	3.424	0.008	.
1	A	190	ARG	CB	29.847	0.038	.
1	A	190	ARG	HB2	1.76	0.006	.
1	A	190	ARG	HB3	1.646	0.009	.
1	A	190	ARG	CG	27.832	0.048	.
1	A	190	ARG	HG2	1.564	0.011	.
1	A	190	ARG	HG3	1.614	0.008	.
1	A	190	ARG	CD	43.509	0.005	.
1	A	190	ARG	HD2	3.23	0.005	.
1	A	190	ARG	HD3	3.23	0.005	.
1	A	190	ARG	C	177.438	0.000	.
1	A	191	GLY	N	112.7	0.026	.
1	A	191	GLY	H	8.688	0.005	.
1	A	191	GLY	CA	46.044	0.000	.
1	A	191	GLY	HA2	4.112	0.016	.
1	A	191	GLY	HA3	4.031	0.012	.
1	A	191	GLY	C	173.27	0.000	.
1	A	192	GLU	N	120.869	0.025	.
1	A	192	GLU	H	7.869	0.003	.
1	A	192	GLU	CA	55.713	0.035	.
1	A	192	GLU	HA	4.442	0.008	.
1	A	192	GLU	CB	32.529	0.047	.
1	A	192	GLU	HB2	2.079	0.007	.
1	A	192	GLU	HB3	1.825	0.006	.
1	A	192	GLU	CG	36.573	0.037	.
1	A	192	GLU	HG2	2.234	0.008	.
1	A	192	GLU	HG3	2.08	0.008	.
1	A	192	GLU	C	174.391	0.000	.
1	A	193	VAL	N	121.232	0.034	.
1	A	193	VAL	H	8.292	0.005	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	193	VAL	CA	60.44	0.028	.
1	A	193	VAL	HA	4.709	0.011	.
1	A	193	VAL	CB	33.438	0.007	.
1	A	193	VAL	HB	1.928	0.007	.
1	A	193	VAL	HG11	0.825	0.009	.
1	A	193	VAL	HG12	0.825	0.009	.
1	A	193	VAL	HG13	0.825	0.009	.
1	A	193	VAL	HG21	0.706	0.008	.
1	A	193	VAL	HG22	0.706	0.008	.
1	A	193	VAL	HG23	0.706	0.008	.
1	A	193	VAL	CG1	22.538	0.063	.
1	A	193	VAL	CG2	21.216	0.041	.
1	A	193	VAL	C	176.908	0.000	.
1	A	194	VAL	N	130.453	0.017	.
1	A	194	VAL	H	8.981	0.005	.
1	A	194	VAL	CA	61.902	0.031	.
1	A	194	VAL	HA	4.349	0.009	.
1	A	194	VAL	CB	33.514	0.063	.
1	A	194	VAL	HB	1.752	0.010	.
1	A	194	VAL	HG11	0.849	0.009	.
1	A	194	VAL	HG12	0.849	0.009	.
1	A	194	VAL	HG13	0.849	0.009	.
1	A	194	VAL	HG21	0.748	0.007	.
1	A	194	VAL	HG22	0.748	0.007	.
1	A	194	VAL	HG23	0.748	0.007	.
1	A	194	VAL	CG1	22.474	0.048	.
1	A	194	VAL	CG2	22.21	0.036	.
1	A	194	VAL	C	173.841	0.000	.
1	A	195	CYS	N	121.453	0.053	.
1	A	195	CYS	H	8.234	0.007	.
1	A	195	CYS	CA	55.397	0.028	.
1	A	195	CYS	HA	5.842	0.009	.
1	A	195	CYS	CB	30.198	0.047	.
1	A	195	CYS	HB2	2.586	0.009	.
1	A	195	CYS	HB3	3.101	0.009	.
1	A	195	CYS	C	173.419	0.000	.
1	A	196	LEU	N	127.867	0.025	.
1	A	196	LEU	H	9.906	0.003	.
1	A	196	LEU	CA	52.966	0.035	.
1	A	196	LEU	HA	4.581	0.010	.
1	A	196	LEU	CB	41.692	0.026	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	196	LEU	HB2	0.95	0.006	.
1	A	196	LEU	HB3	1.629	0.010	.
1	A	196	LEU	CG	27.903	0.036	.
1	A	196	LEU	HG	0.348	0.007	.
1	A	196	LEU	HD11	0.661	0.013	.
1	A	196	LEU	HD12	0.661	0.013	.
1	A	196	LEU	HD13	0.661	0.013	.
1	A	196	LEU	HD21	-0.653	0.006	.
1	A	196	LEU	HD22	-0.653	0.006	.
1	A	196	LEU	HD23	-0.653	0.006	.
1	A	196	LEU	CD1	27.052	0.057	.
1	A	196	LEU	CD2	21.832	0.034	.
1	A	196	LEU	C	175.809	0.000	.
1	A	197	TYR	N	129.672	0.033	.
1	A	197	TYR	H	9.041	0.010	.
1	A	197	TYR	CA	58.509	0.058	.
1	A	197	TYR	HA	4.674	0.009	.
1	A	197	TYR	CB	40.972	0.030	.
1	A	197	TYR	HB2	2.443	0.009	.
1	A	197	TYR	HB3	2.367	0.014	.
1	A	197	TYR	HD1	6.625	0.010	.
1	A	197	TYR	HD2	6.625	0.010	.
1	A	197	TYR	HE1	6.412	0.009	.
1	A	197	TYR	HE2	6.412	0.009	.
1	A	197	TYR	CE2	117.033	0.029	.
1	A	197	TYR	CD2	131.923	0.048	.
1	A	197	TYR	C	176.104	0.000	.
1	A	198	VAL	N	121.515	0.026	.
1	A	198	VAL	H	8.247	0.006	.
1	A	198	VAL	CA	61.155	0.035	.
1	A	198	VAL	HA	4.637	0.008	.
1	A	198	VAL	CB	32.895	0.019	.
1	A	198	VAL	HB	2.001	0.006	.
1	A	198	VAL	HG11	0.673	0.008	.
1	A	198	VAL	HG12	0.673	0.008	.
1	A	198	VAL	HG13	0.673	0.008	.
1	A	198	VAL	HG21	0.52	0.006	.
1	A	198	VAL	HG22	0.52	0.006	.
1	A	198	VAL	HG23	0.52	0.006	.
1	A	198	VAL	CG1	22.822	0.040	.
1	A	198	VAL	CG2	20.305	0.069	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	198	VAL	C	174.661	0.000	.
1	A	199	THR	N	114.726	0.019	.
1	A	199	THR	H	7.363	0.002	.
1	A	199	THR	CA	58.802	0.027	.
1	A	199	THR	HA	4.566	0.011	.
1	A	199	THR	CB	70.775	0.040	.
1	A	199	THR	HB	4.404	0.009	.
1	A	199	THR	HG21	1.206	0.012	.
1	A	199	THR	HG22	1.206	0.012	.
1	A	199	THR	HG23	1.206	0.012	.
1	A	199	THR	CG2	22.196	0.027	.
1	A	199	THR	C	173.576	0.000	.
1	A	200	GLY	N	106.923	0.017	.
1	A	200	GLY	H	8.788	0.007	.
1	A	200	GLY	CA	44.773	0.038	.
1	A	200	GLY	HA2	4.436	0.010	.
1	A	200	GLY	HA3	4.141	0.007	.
1	A	200	GLY	C	173.226	0.000	.
1	A	201	SER	N	113.184	0.038	.
1	A	201	SER	H	7.686	0.004	.
1	A	201	SER	CA	56.813	0.014	.
1	A	201	SER	HA	4.914	0.010	.
1	A	201	SER	CB	67.539	0.022	.
1	A	201	SER	HB2	3.708	0.010	.
1	A	201	SER	HB3	4.517	0.011	.
1	A	201	SER	C	173.226	0.000	.
1	A	202	GLY	CA	45.655	0.045	.
1	A	202	GLY	HA2	3.812	0.007	.
1	A	202	GLY	HA3	4.006	0.004	.
1	A	202	GLY	C	173.965	0.000	.
1	A	203	GLY	N	106.761	0.007	.
1	A	203	GLY	H	7.65	0.001	.
1	A	203	GLY	CA	45.02	0.000	.
1	A	203	GLY	HA2	3.747	0.013	.
1	A	203	GLY	HA3	4.044	0.013	.
1	A	203	GLY	C	173.832	0.000	.
1	A	204	LYS	N	121.554	0.012	.
1	A	204	LYS	H	7.724	0.003	.
1	A	204	LYS	CA	54.71	0.030	.
1	A	204	LYS	HA	4.552	0.008	.
1	A	204	LYS	CB	32.997	0.002	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	204	LYS	HB2	1.874	0.009	.
1	A	204	LYS	HB3	1.748	0.009	.
1	A	204	LYS	CG	24.617	0.073	.
1	A	204	LYS	HG2	1.362	0.011	.
1	A	204	LYS	HG3	1.362	0.011	.
1	A	204	LYS	CD	28.929	0.053	.
1	A	204	LYS	HD2	1.647	0.009	.
1	A	204	LYS	HD3	1.651	0.007	.
1	A	204	LYS	CE	42.151	0.041	.
1	A	204	LYS	HE2	3.033	0.009	.
1	A	204	LYS	HE3	2.975	0.010	.
1	A	204	LYS	C	175.516	0.000	.
1	A	205	LEU	N	122.967	0.035	.
1	A	205	LEU	H	8.191	0.006	.
1	A	205	LEU	CA	54.37	0.038	.
1	A	205	LEU	HA	4.726	0.012	.
1	A	205	LEU	CB	44.054	0.036	.
1	A	205	LEU	HB2	0.903	0.009	.
1	A	205	LEU	HB3	1.575	0.014	.
1	A	205	LEU	CG	26.934	0.033	.
1	A	205	LEU	HG	1.533	0.012	.
1	A	205	LEU	HD11	0.726	0.010	.
1	A	205	LEU	HD12	0.726	0.010	.
1	A	205	LEU	HD13	0.726	0.010	.
1	A	205	LEU	HD21	0.652	0.010	.
1	A	205	LEU	HD22	0.652	0.010	.
1	A	205	LEU	HD23	0.652	0.010	.
1	A	205	LEU	CD1	26.255	0.014	.
1	A	205	LEU	CD2	23.415	0.050	.
1	A	205	LEU	C	176.851	0.000	.
1	A	206	ALA	N	125.2	0.022	.
1	A	206	ALA	H	8.841	0.003	.
1	A	206	ALA	CA	49.164	0.012	.
1	A	206	ALA	HA	4.921	0.009	.
1	A	206	ALA	HB1	1.202	0.010	.
1	A	206	ALA	HB2	1.202	0.010	.
1	A	206	ALA	HB3	1.202	0.010	.
1	A	206	ALA	CB	19.483	0.042	.
1	A	206	ALA	C	176.851	0.000	.
1	A	207	PRO	CD	49.828	0.035	.
1	A	207	PRO	CA	60.178	0.042	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	207	PRO	HA	5.231	0.007	.
1	A	207	PRO	CB	32.141	0.050	.
1	A	207	PRO	HB2	1.547	0.009	.
1	A	207	PRO	HB3	1.639	0.008	.
1	A	207	PRO	CG	27.081	0.025	.
1	A	207	PRO	HG2	2.162	0.008	.
1	A	207	PRO	HG3	2.162	0.008	.
1	A	207	PRO	HD2	3.733	0.011	.
1	A	207	PRO	HD3	3.411	0.009	.
1	A	207	PRO	C	176.022	0.000	.
1	A	208	VAL	N	128.613	0.014	.
1	A	208	VAL	H	9.061	0.007	.
1	A	208	VAL	CA	61.458	0.058	.
1	A	208	VAL	HA	4.067	0.007	.
1	A	208	VAL	CB	37.606	0.020	.
1	A	208	VAL	HB	1.926	0.008	.
1	A	208	VAL	HG11	0.876	0.012	.
1	A	208	VAL	HG12	0.876	0.012	.
1	A	208	VAL	HG13	0.876	0.012	.
1	A	208	VAL	HG21	1.031	0.007	.
1	A	208	VAL	HG22	1.031	0.007	.
1	A	208	VAL	HG23	1.031	0.007	.
1	A	208	VAL	CG1	22.406	0.049	.
1	A	208	VAL	CG2	21.457	0.047	.
1	A	208	VAL	C	175.403	0.000	.
1	A	209	TRP	N	126.012	0.022	.
1	A	209	TRP	H	8.534	0.003	.
1	A	209	TRP	CA	56.713	0.040	.
1	A	209	TRP	HA	5.285	0.007	.
1	A	209	TRP	CB	30.646	0.033	.
1	A	209	TRP	HB2	3.155	0.008	.
1	A	209	TRP	HB3	2.803	0.007	.
1	A	209	TRP	CD1	127.59	0.000	.
1	A	209	TRP	CE3	121.364	0.029	.
1	A	209	TRP	NE1	127.52	0.030	.
1	A	209	TRP	HD1	7.121	0.010	.
1	A	209	TRP	HE3	7.363	0.013	.
1	A	209	TRP	CZ3	122.05	0.000	.
1	A	209	TRP	CZ2	115.198	0.002	.
1	A	209	TRP	HE1	10.105	0.003	.
1	A	209	TRP	HZ3	6.633	0.010	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	209	TRP	CH2	122.206	0.041	.
1	A	209	TRP	HZ2	7.379	0.008	.
1	A	209	TRP	HH2	6.714	0.005	.
1	A	209	TRP	C	176.699	0.000	.
1	A	210	VAL	N	127.659	0.020	.
1	A	210	VAL	H	10.163	0.004	.
1	A	210	VAL	CA	62.663	0.034	.
1	A	210	VAL	HA	4.157	0.011	.
1	A	210	VAL	CB	33.641	0.054	.
1	A	210	VAL	HB	1.815	0.006	.
1	A	210	VAL	HG11	0.129	0.006	.
1	A	210	VAL	HG12	0.129	0.006	.
1	A	210	VAL	HG13	0.129	0.006	.
1	A	210	VAL	HG21	0.566	0.006	.
1	A	210	VAL	HG22	0.566	0.006	.
1	A	210	VAL	HG23	0.566	0.006	.
1	A	210	VAL	CG1	21.518	0.034	.
1	A	210	VAL	CG2	19.245	0.049	.
1	A	210	VAL	C	174.905	0.000	.
1	A	211	LYS	N	129.212	0.021	.
1	A	211	LYS	H	8.647	0.005	.
1	A	211	LYS	CA	54.34	0.033	.
1	A	211	LYS	HA	4.86	0.012	.
1	A	211	LYS	CB	36.511	0.035	.
1	A	211	LYS	HB2	1.683	0.005	.
1	A	211	LYS	HB3	1.855	0.010	.
1	A	211	LYS	CG	24.539	0.044	.
1	A	211	LYS	HG2	1.402	0.009	.
1	A	211	LYS	HG3	1.402	0.009	.
1	A	211	LYS	CD	29.537	0.011	.
1	A	211	LYS	HD2	1.546	0.009	.
1	A	211	LYS	HD3	1.546	0.009	.
1	A	211	LYS	CE	41.469	0.049	.
1	A	211	LYS	HE2	2.844	0.007	.
1	A	211	LYS	HE3	2.89	0.009	.
1	A	211	LYS	C	174.692	0.000	.
1	A	212	ARG	N	123.764	0.056	.
1	A	212	ARG	H	9.164	0.003	.
1	A	212	ARG	CA	54.868	0.057	.
1	A	212	ARG	HA	4.769	0.010	.
1	A	212	ARG	CB	30.3	0.007	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	212	ARG	HB2	2.031	0.010	.
1	A	212	ARG	HB3	1.743	0.015	.
1	A	212	ARG	CG	20.788	0.000	.
1	A	212	ARG	HG2	1.037	0.001	.
1	A	212	ARG	HG3	1.037	0.001	.
1	A	212	ARG	CD	44.055	0.009	.
1	A	212	ARG	HD2	3.379	0.003	.
1	A	212	ARG	HD3	3.499	0.005	.
1	A	212	ARG	C	174.692	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	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
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	.
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	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
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	.
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	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	222	HIS	HB3	3.015	0.001	.

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	191	0.26 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	173	0.15 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	181	0.46 ± 0.07	None needed (< 0.5 ppm)
^{15}N	171	-0.56 ± 0.36	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 94%, i.e. 929 atoms were assigned a chemical shift out of a possible 992. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	374/390 (96%)	155/159 (97%)	152/160 (95%)	67/71 (94%)
Sidechain	507/536 (95%)	340/351 (97%)	158/170 (93%)	9/15 (60%)
Aromatic	48/66 (73%)	31/31 (100%)	17/35 (49%)	0/0 (—%)
Overall	929/992 (94%)	526/541 (97%)	327/365 (90%)	76/86 (88%)

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:

