



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 03:05 PM UTC

PDB ID : 8OVL / pdb_00008ovl
BMRB ID : 34812
Title : NMR solution structure of the heavy metal binding domain of P1B-ATPase
LpCopA.
Authors : Nielsen, T.J.
Deposited on : 2023-04-26

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

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

A user guide is available at

<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 : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

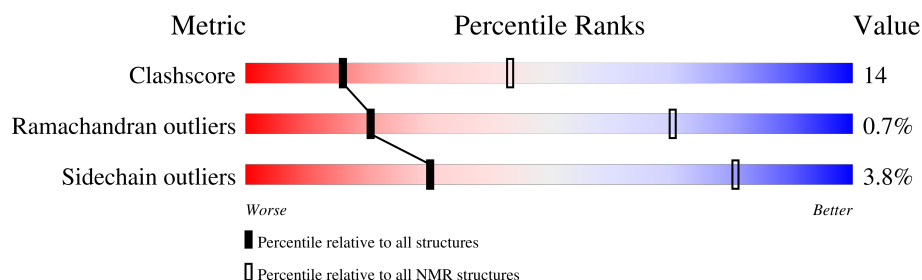
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 4%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	83	

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 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:3-A:32 (30)	0.32	4

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 5 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 512 atoms, of which 255 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Copper-translocating P-type ATPase.

Mol	Chain	Residues	Atoms						Trace
1	A	35	Total	C	H	N	O	S	0
			512	162	255	43	47	5	

There is a discrepancy between the modelled and reference sequences:

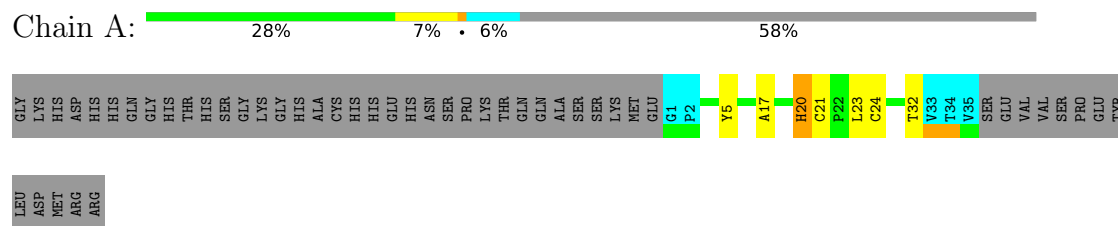
Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	GLY	-	expression tag	UNP Q8RNP6

4 Residue-property plots

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: Copper-translocating P-type ATPase

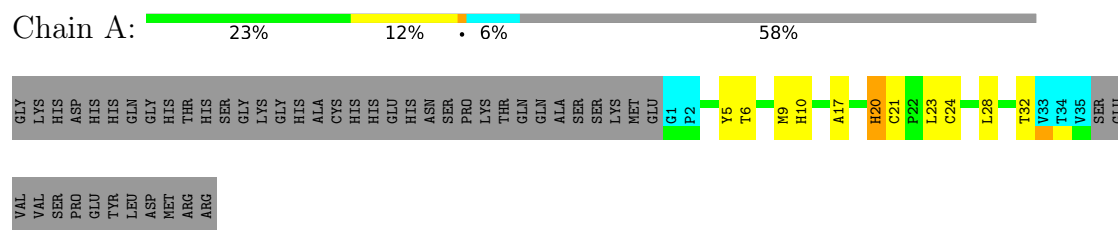


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

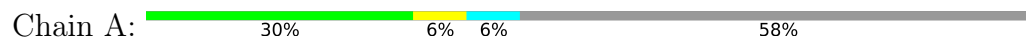
4.2.1 Score per residue for model 1

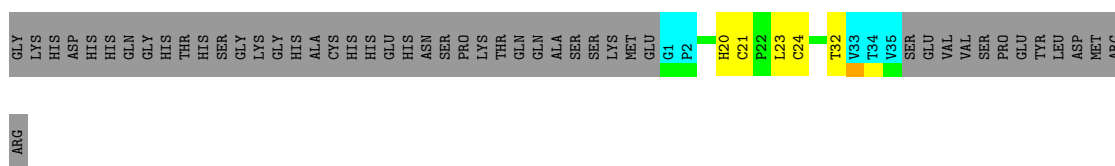
- Molecule 1: Copper-translocating P-type ATPase



4.2.2 Score per residue for model 2

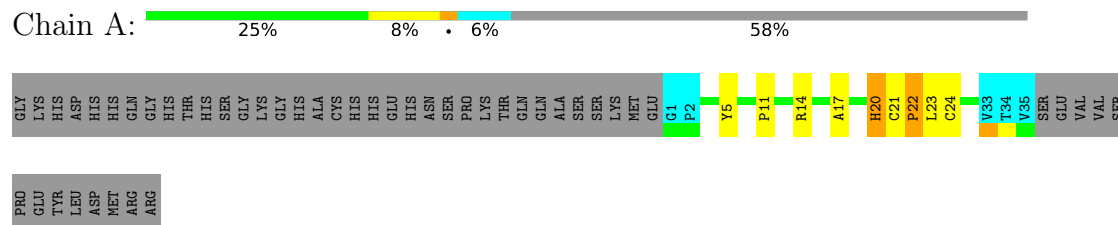
- Molecule 1: Copper-translocating P-type ATPase





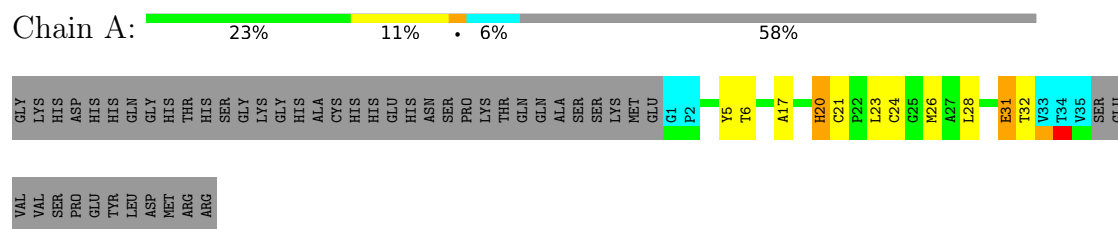
4.2.3 Score per residue for model 3

- Molecule 1: Copper-translocating P-type ATPase



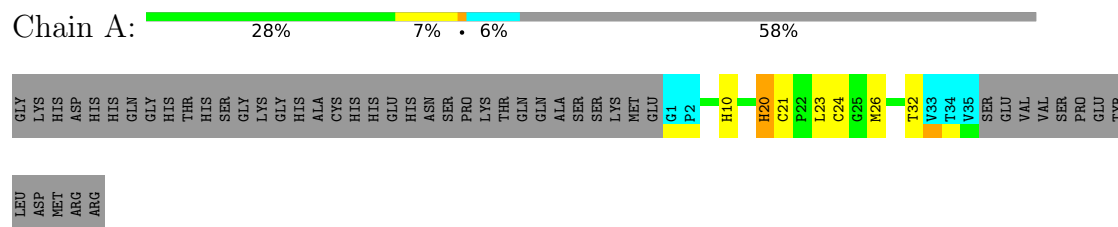
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Copper-translocating P-type ATPase



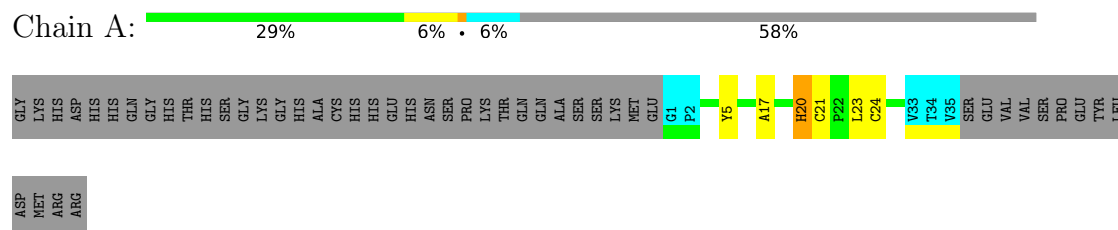
4.2.5 Score per residue for model 5

- Molecule 1: Copper-translocating P-type ATPase



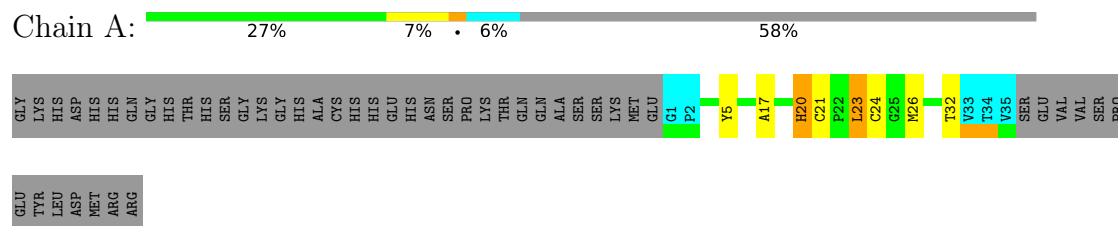
4.2.6 Score per residue for model 6

- Molecule 1: Copper-translocating P-type ATPase



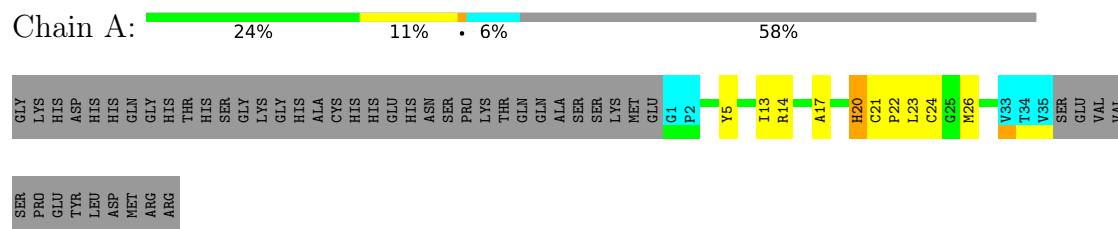
4.2.7 Score per residue for model 7

- Molecule 1: Copper-translocating P-type ATPase



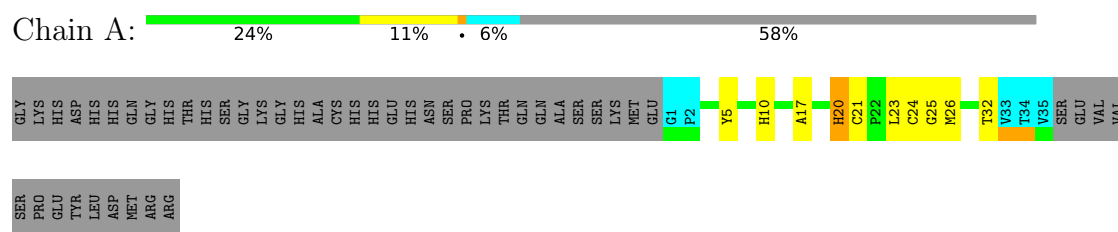
4.2.8 Score per residue for model 8

- Molecule 1: Copper-translocating P-type ATPase



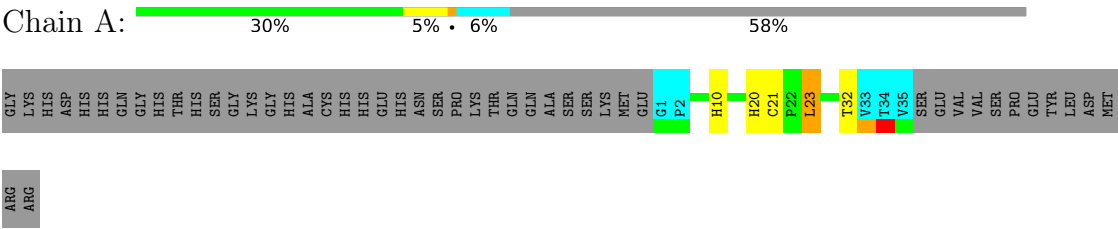
4.2.9 Score per residue for model 9

- Molecule 1: Copper-translocating P-type ATPase



4.2.10 Score per residue for model 10

- Molecule 1: Copper-translocating P-type ATPase



5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 10 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	
X-PLOR NIH	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	813
Number of shifts mapped to atoms	20
Number of unparsed shifts	0
Number of shifts with mapping errors	793
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	4%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.84±0.03	0±0/233 (0.0± 0.0%)	1.09±0.02	0±1/320 (0.1± 0.2%)
All	All	0.84	0/2330 (0.0%)	1.09	3/3200 (0.1%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	10	HIS	CA-CB-CG	-5.43	108.37	113.80	5	1
1	A	20	HIS	CA-CB-CG	-5.24	108.56	113.80	8	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	225	220	218	6±1
All	All	2250	2200	2180	64

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:LEU:O	1:A:23:LEU:HD22	0.79	1.77	10	1
1:A:23:LEU:HD22	1:A:23:LEU:C	0.60	2.21	10	1
1:A:23:LEU:C	1:A:23:LEU:HD12	0.58	2.23	8	1
1:A:20:HIS:CD2	1:A:25:GLY:O	0.58	2.56	9	1
1:A:23:LEU:HD12	1:A:24:CYS:N	0.57	2.13	1	9
1:A:11:PRO:O	1:A:14:ARG:CZ	0.53	2.57	3	1
1:A:5:TYR:CD1	1:A:17:ALA:C	0.52	2.88	4	7
1:A:23:LEU:HD12	1:A:23:LEU:C	0.52	2.30	2	6
1:A:21:CYS:SG	1:A:24:CYS:SG	0.50	3.03	6	1
1:A:9:MET:SD	1:A:9:MET:O	0.50	2.70	1	1
1:A:11:PRO:O	1:A:14:ARG:NH1	0.49	2.45	3	1
1:A:24:CYS:C	1:A:26:MET:H	0.48	2.17	7	5
1:A:9:MET:SD	1:A:10:HIS:CE1	0.48	3.07	1	1
1:A:20:HIS:O	1:A:21:CYS:C	0.48	2.57	9	10
1:A:31:GLU:CD	1:A:32:THR:N	0.48	2.72	4	1
1:A:31:GLU:CD	1:A:32:THR:H	0.48	2.17	4	1
1:A:23:LEU:CD1	1:A:23:LEU:C	0.47	2.88	7	2
1:A:31:GLU:OE1	1:A:32:THR:N	0.46	2.48	4	1
1:A:10:HIS:ND1	1:A:23:LEU:HD11	0.46	2.25	10	1
1:A:23:LEU:C	1:A:23:LEU:CD1	0.46	2.89	9	5
1:A:6:THR:C	1:A:28:LEU:HD23	0.45	2.37	1	2
1:A:13:ILE:HG21	1:A:21:CYS:SG	0.44	2.51	8	1
1:A:23:LEU:C	1:A:23:LEU:CD2	0.43	2.91	10	1
1:A:9:MET:SD	1:A:9:MET:C	0.42	3.02	1	1
1:A:21:CYS:O	1:A:22:PRO:C	0.42	2.63	3	1
1:A:24:CYS:C	1:A:26:MET:N	0.41	2.79	7	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	30/83 (36%)	26±1 (86±3%)	4±1 (14±4%)	0±0 (1±1%)	20	70
All	All	300/830 (36%)	257 (86%)	41 (14%)	2 (1%)	20	70

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	22	PRO	2

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	26/72 (36%)	25±1 (96±3%)	1±1 (4±3%)	30	81
All	All	260/720 (36%)	250 (96%)	10 (4%)	30	81

All 4 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	20	HIS	6
1	A	23	LEU	2
1	A	31	GLU	1
1	A	10	HIS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 4% for the well-defined parts and 5% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

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	813
Number of shifts mapped to atoms	20
Number of unparsed shifts	0
Number of shifts with mapping errors	793
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. All 793 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	LYS	N	120.06	0.072	1
1	A	2	LYS	H	8.81	0.020	1
1	A	2	LYS	CA	57.27	0.162	1
1	A	2	LYS	HA	4.24	0.025	1
1	A	2	LYS	CB	33.11	0.160	1
1	A	2	LYS	HB2	1.7	0.027	1
1	A	2	LYS	CG	24.84	0.184	1
1	A	2	LYS	HG2	1.36	0.024	1
1	A	2	LYS	CD	29.26	0.189	1
1	A	2	LYS	HD2	1.68	0.026	1
1	A	2	LYS	CE	42.12	0.185	1
1	A	2	LYS	HE2	2.98	0.028	1
1	A	2	LYS	C	176.99	0.143	1
1	A	3	HIS	N	118.44	0.071	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	HIS	H	8.9	0.020	1
1	A	3	HIS	CA	54.56	0.255	1
1	A	3	HIS	HA	4.82	0.035	1
1	A	3	HIS	CB	28.76	0.187	1
1	A	3	HIS	HB2	3.18	0.046	1
1	A	3	HIS	C	174.09	0.143	1
1	A	4	ASP	N	120.48	0.072	1
1	A	4	ASP	H	8.27	0.020	1
1	A	4	ASP	CA	54.41	0.165	1
1	A	4	ASP	HA	4.58	0.025	1
1	A	4	ASP	CB	40.9	0.159	1
1	A	4	ASP	HB2	2.65	0.024	1
1	A	4	ASP	C	175.97	0.143	1
1	A	5	HIS	N	118.9	0.072	1
1	A	5	HIS	H	8.78	0.020	1
1	A	5	HIS	CA	55.12	0.185	1
1	A	5	HIS	HA	4.74	0.031	1
1	A	5	HIS	CB	28.72	0.187	1
1	A	5	HIS	HB2	3.22	0.033	1
1	A	5	HIS	C	174.42	0.143	1
1	A	6	HIS	N	120.09	0.072	1
1	A	6	HIS	H	8.8	0.020	1
1	A	6	HIS	CA	55.72	0.194	1
1	A	6	HIS	HA	4.71	0.035	1
1	A	6	HIS	CB	28.86	0.189	1
1	A	6	HIS	HB2	3.22	0.034	1
1	A	6	HIS	C	174.39	0.143	1
1	A	7	GLN	N	122.29	0.072	1
1	A	7	GLN	H	8.74	0.020	1
1	A	7	GLN	CA	56.02	0.182	1
1	A	7	GLN	HA	4.36	0.031	1
1	A	7	GLN	CB	29.53	0.213	1
1	A	7	GLN	HB2	2.06	0.032	1
1	A	7	GLN	CG	33.72	0.202	1
1	A	7	GLN	HG2	2.39	0.029	1
1	A	7	GLN	C	176.38	0.143	1
1	A	8	GLY	N	110.59	0.072	1
1	A	8	GLY	H	8.68	0.020	1
1	A	8	GLY	CA	45.26	0.187	1
1	A	8	GLY	HA2	3.97	0.042	1
1	A	8	GLY	HA3	4.01	0.046	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	GLY	C	173.82	0.143	1
1	A	9	HIS	N	117.94	0.072	1
1	A	9	HIS	H	8.68	0.020	1
1	A	9	HIS	CA	55.13	0.222	1
1	A	9	HIS	HA	4.85	0.037	1
1	A	9	HIS	CB	29.27	0.187	1
1	A	9	HIS	HB2	3.23	0.035	1
1	A	9	HIS	C	174.92	0.143	1
1	A	10	THR	N	115.53	0.072	1
1	A	10	THR	H	8.44	0.020	1
1	A	10	THR	CA	62.25	0.167	1
1	A	10	THR	HA	4.34	0.034	1
1	A	10	THR	CB	70.07	0.167	1
1	A	10	THR	HB	4.26	0.042	1
1	A	10	THR	CG2	21.72	0.195	1
1	A	10	THR	HG21	1.19	0.026	1
1	A	10	THR	HG22	1.19	0.026	1
1	A	10	THR	HG23	1.19	0.026	1
1	A	10	THR	C	174.47	0.143	1
1	A	11	HIS	N	120.93	0.072	1
1	A	11	HIS	H	8.9	0.020	1
1	A	11	HIS	CA	55.23	0.198	1
1	A	11	HIS	HA	4.82	0.029	1
1	A	11	HIS	CB	29.14	0.170	1
1	A	11	HIS	HB2	3.26	0.027	1
1	A	11	HIS	C	174.45	0.143	1
1	A	12	SER	N	117.78	0.072	1
1	A	12	SER	H	8.63	0.020	1
1	A	12	SER	CA	58.5	0.171	1
1	A	12	SER	HA	4.52	0.030	1
1	A	12	SER	CB	64.4	0.195	1
1	A	12	SER	HB2	3.88	0.034	1
1	A	12	SER	C	175.02	0.143	1
1	A	13	GLY	N	111.11	0.072	1
1	A	13	GLY	H	8.71	0.020	1
1	A	13	GLY	CA	45.23	0.187	1
1	A	13	GLY	HA2	4.04	0.041	1
1	A	13	GLY	HA3	4.07	0.042	1
1	A	13	GLY	C	174.2	0.143	1
1	A	14	LYS	N	120.74	0.072	1
1	A	14	LYS	H	8.48	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	14	LYS	CA	56.55	0.170	1
1	A	14	LYS	HA	4.36	0.027	1
1	A	14	LYS	CB	33.17	0.164	1
1	A	14	LYS	HB2	1.82	0.026	1
1	A	14	LYS	CG	24.83	0.186	1
1	A	14	LYS	HG2	1.46	0.027	1
1	A	14	LYS	CD	29.25	0.191	1
1	A	14	LYS	HD2	1.73	0.046	1
1	A	14	LYS	CE	42.16	0.187	1
1	A	14	LYS	HE2	3.0	0.028	1
1	A	14	LYS	C	177.52	0.143	1
1	A	15	GLY	N	109.97	0.072	1
1	A	15	GLY	H	8.66	0.020	1
1	A	15	GLY	CA	45.27	0.188	1
1	A	15	GLY	HA2	3.93	0.042	1
1	A	15	GLY	HA3	3.96	0.047	1
1	A	15	GLY	C	173.96	0.143	1
1	A	16	HIS	N	117.89	0.072	1
1	A	16	HIS	H	8.54	0.020	1
1	A	16	HIS	CA	55.05	0.219	1
1	A	16	HIS	HA	4.76	0.031	1
1	A	16	HIS	CB	29.29	0.187	1
1	A	16	HIS	HB2	3.23	0.033	1
1	A	16	HIS	C	174.26	0.143	1
1	A	18	CYS	N	119.26	0.072	1
1	A	18	CYS	H	8.59	0.020	1
1	A	18	CYS	CA	58.64	0.202	1
1	A	18	CYS	HA	4.47	0.025	1
1	A	18	CYS	CB	28.21	0.169	1
1	A	18	CYS	HB2	2.87	0.025	1
1	A	18	CYS	C	174.38	0.143	1
1	A	19	HIS	N	121.48	0.072	1
1	A	19	HIS	H	8.84	0.020	1
1	A	19	HIS	CA	55.29	0.199	1
1	A	19	HIS	HA	4.74	0.032	1
1	A	19	HIS	CB	28.99	0.188	1
1	A	19	HIS	HB2	3.22	0.034	1
1	A	19	HIS	C	174.05	0.143	1
1	A	21	GLU	N	122.42	0.072	1
1	A	21	GLU	H	8.8	0.020	1
1	A	21	GLU	CA	56.19	0.187	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	21	GLU	HA	4.31	0.031	1
1	A	21	GLU	CB	29.73	0.195	1
1	A	21	GLU	HB2	1.97	0.031	1
1	A	21	GLU	CG	34.18	0.287	1
1	A	21	GLU	HG2	2.36	0.031	1
1	A	21	GLU	C	176.11	0.143	1
1	A	22	HIS	N	119.85	0.072	1
1	A	22	HIS	H	8.9	0.020	1
1	A	22	HIS	CA	55.59	0.304	1
1	A	22	HIS	HA	4.75	0.031	1
1	A	22	HIS	CB	29.16	0.187	1
1	A	22	HIS	HB2	3.24	0.032	1
1	A	22	HIS	C	174.1	0.143	1
1	A	23	ASN	N	120.79	0.072	1
1	A	23	ASN	H	8.74	0.020	1
1	A	23	ASN	CA	53.46	0.193	1
1	A	23	ASN	HA	4.79	0.029	1
1	A	23	ASN	CB	39.17	0.160	1
1	A	23	ASN	HB2	2.77	0.025	1
1	A	23	ASN	C	174.94	0.143	1
1	A	24	SER	N	118.13	0.072	1
1	A	24	SER	H	8.63	0.020	1
1	A	24	SER	CA	56.64	0.192	1
1	A	24	SER	HA	4.8	0.030	1
1	A	24	SER	CB	63.27	0.192	1
1	A	24	SER	HB2	3.87	0.036	1
1	A	25	PRO	CA	63.28	0.181	1
1	A	25	PRO	HA	4.47	0.037	1
1	A	25	PRO	CB	32.23	0.183	1
1	A	25	PRO	HB2	2.32	0.040	1
1	A	25	PRO	CG	27.43	0.209	1
1	A	25	PRO	HG2	1.99	0.038	1
1	A	25	PRO	CD	50.7	0.313	1
1	A	25	PRO	HD2	3.78	0.049	1
1	A	25	PRO	C	177.1	0.143	1
1	A	26	LYS	N	121.68	0.072	1
1	A	26	LYS	H	8.64	0.020	1
1	A	26	LYS	CA	56.63	0.172	1
1	A	26	LYS	HA	4.37	0.028	1
1	A	26	LYS	CB	32.84	0.214	1
1	A	26	LYS	HB2	1.83	0.026	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	26	LYS	CG	24.87	0.185	1
1	A	26	LYS	HG2	1.47	0.027	1
1	A	26	LYS	CD	29.25	0.191	1
1	A	26	LYS	HD2	1.73	0.047	1
1	A	26	LYS	CE	42.19	0.187	1
1	A	26	LYS	HE2	3.01	0.028	1
1	A	26	LYS	C	177.17	0.143	1
1	A	27	THR	N	115.61	0.072	1
1	A	27	THR	H	8.3	0.020	1
1	A	27	THR	CA	62.15	0.161	1
1	A	27	THR	HA	4.33	0.029	1
1	A	27	THR	CB	70.04	0.163	1
1	A	27	THR	HB	4.26	0.036	1
1	A	27	THR	CG2	21.75	0.190	1
1	A	27	THR	HG21	1.2	0.025	1
1	A	27	THR	HG22	1.2	0.025	1
1	A	27	THR	HG23	1.2	0.025	1
1	A	27	THR	C	174.58	0.143	1
1	A	28	GLN	N	122.94	0.072	1
1	A	28	GLN	H	8.63	0.020	1
1	A	28	GLN	CA	55.97	0.179	1
1	A	28	GLN	HA	4.37	0.031	1
1	A	28	GLN	CB	29.59	0.199	1
1	A	28	GLN	HB2	2.07	0.029	1
1	A	28	GLN	CG	33.74	0.210	1
1	A	28	GLN	HG2	2.39	0.031	1
1	A	28	GLN	C	176.01	0.143	1
1	A	29	GLN	N	122.49	0.072	1
1	A	29	GLN	H	8.66	0.020	1
1	A	29	GLN	CA	56.01	0.188	1
1	A	29	GLN	HA	4.86	0.084	1
1	A	29	GLN	CB	29.55	0.171	1
1	A	29	GLN	HB2	2.07	0.035	1
1	A	29	GLN	CG	33.74	0.244	1
1	A	29	GLN	HG2	2.4	0.043	1
1	A	29	GLN	C	176.0	0.143	1
1	A	30	ALA	N	126.06	0.072	1
1	A	30	ALA	H	8.67	0.020	1
1	A	30	ALA	CA	52.72	0.171	1
1	A	30	ALA	HA	4.36	0.026	1
1	A	30	ALA	CB	19.07	0.186	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	30	ALA	HB1	1.41	0.026	1
1	A	30	ALA	HB2	1.41	0.026	1
1	A	30	ALA	HB3	1.41	0.026	1
1	A	30	ALA	C	178.12	0.143	1
1	A	31	SER	N	115.31	0.072	1
1	A	31	SER	H	8.55	0.020	1
1	A	31	SER	CA	58.55	0.195	1
1	A	31	SER	HA	4.51	0.033	1
1	A	31	SER	CB	64.12	0.178	1
1	A	31	SER	HB2	3.91	0.027	1
1	A	31	SER	C	174.92	0.143	1
1	A	32	SER	N	117.93	0.072	1
1	A	32	SER	H	8.52	0.020	1
1	A	32	SER	CA	58.55	0.194	1
1	A	32	SER	HA	4.49	0.027	1
1	A	32	SER	CB	64.12	0.248	1
1	A	32	SER	HB2	3.9	0.026	1
1	A	32	SER	C	174.61	0.142	1
1	A	33	LYS	N	122.9	0.073	1
1	A	33	LYS	H	8.43	0.020	1
1	A	33	LYS	CA	56.46	0.173	1
1	A	33	LYS	HA	4.36	0.028	1
1	A	33	LYS	CB	33.0	0.186	1
1	A	33	LYS	HB2	1.82	0.029	1
1	A	33	LYS	CG	24.82	0.188	1
1	A	33	LYS	HG2	1.44	0.030	1
1	A	33	LYS	CD	29.22	0.192	1
1	A	33	LYS	HD2	1.74	0.041	1
1	A	33	LYS	CE	42.14	0.259	1
1	A	33	LYS	HE2	2.96	0.044	1
1	A	33	LYS	C	176.59	0.143	1
1	A	34	MET	N	121.61	0.072	1
1	A	34	MET	H	8.49	0.020	1
1	A	34	MET	CA	55.63	0.172	1
1	A	34	MET	HA	4.5	0.030	1
1	A	34	MET	CB	32.75	0.218	1
1	A	34	MET	HB2	2.07	0.035	1
1	A	34	MET	CG	32.0	0.192	1
1	A	34	MET	HG2	2.57	0.027	1
1	A	34	MET	CE	17.06	0.227	1
1	A	34	MET	HE1	2.07	0.052	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	34	MET	HE2	2.07	0.052	1
1	A	34	MET	HE3	2.07	0.052	1
1	A	34	MET	C	176.19	0.143	1
1	A	35	GLU	N	122.22	0.072	1
1	A	35	GLU	H	8.56	0.020	1
1	A	35	GLU	CA	55.96	0.171	1
1	A	35	GLU	HA	4.45	0.028	1
1	A	35	GLU	CB	29.64	0.163	1
1	A	35	GLU	HB2	2.04	0.032	1
1	A	35	GLU	CG	33.66	0.236	1
1	A	35	GLU	HG2	2.44	0.027	1
1	A	35	GLU	C	176.23	0.143	1
1	A	36	GLY	N	110.16	0.072	1
1	A	36	GLY	H	8.41	0.020	1
1	A	36	GLY	CA	44.55	0.231	1
1	A	36	GLY	HA2	4.1	0.051	1
1	A	36	GLY	HA3	4.14	0.057	1
1	A	37	PRO	CA	63.1	0.183	1
1	A	37	PRO	HA	4.49	0.031	1
1	A	37	PRO	CB	32.07	0.160	1
1	A	37	PRO	HB2	1.94	0.039	1
1	A	37	PRO	HB3	2.28	0.035	1
1	A	37	PRO	CG	27.45	0.184	1
1	A	37	PRO	HG2	2.0	0.042	1
1	A	37	PRO	HG3	1.97	0.045	1
1	A	37	PRO	CD	49.85	0.178	1
1	A	37	PRO	HD3	3.64	0.031	1
1	A	37	PRO	HD2	3.64	0.035	1
1	A	37	PRO	C	176.32	0.143	1
1	A	38	ILE	N	121.22	0.071	1
1	A	38	ILE	H	8.32	0.020	1
1	A	38	ILE	CA	60.69	0.162	1
1	A	38	ILE	HA	4.31	0.030	1
1	A	38	ILE	CB	39.52	0.159	1
1	A	38	ILE	HB	1.65	0.026	1
1	A	38	ILE	CG1	27.68	0.223	1
1	A	38	ILE	HG12	1.46	0.031	1
1	A	38	ILE	HG13	1.1	0.085	1
1	A	38	ILE	CG2	17.52	0.215	1
1	A	38	ILE	HG21	0.43	0.035	1
1	A	38	ILE	HG22	0.43	0.035	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	38	ILE	HG23	0.43	0.035	1
1	A	38	ILE	CD1	12.82	0.220	1
1	A	38	ILE	HD11	0.77	0.032	1
1	A	38	ILE	HD12	0.77	0.032	1
1	A	38	ILE	HD13	0.77	0.032	1
1	A	38	ILE	C	176.0	0.143	1
1	A	39	VAL	N	125.24	0.072	1
1	A	39	VAL	H	8.48	0.020	1
1	A	39	VAL	CA	60.69	0.161	1
1	A	39	VAL	HA	4.34	0.025	1
1	A	39	VAL	CB	34.66	0.161	1
1	A	39	VAL	HB	1.82	0.030	1
1	A	39	VAL	CG1	21.12	0.219	1
1	A	39	VAL	CG2	21.12	0.219	1
1	A	39	VAL	HG11	0.81	0.030	1
1	A	39	VAL	HG12	0.81	0.030	1
1	A	39	VAL	HG13	0.81	0.030	1
1	A	39	VAL	HG21	0.8	0.053	1
1	A	39	VAL	HG22	0.8	0.053	1
1	A	39	VAL	HG23	0.8	0.053	1
1	A	39	VAL	C	173.36	0.143	1
1	A	40	TYR	N	123.45	0.077	1
1	A	40	TYR	H	9.25	0.020	1
1	A	40	TYR	CA	57.62	0.168	1
1	A	40	TYR	HA	4.72	0.029	1
1	A	40	TYR	CB	39.91	0.160	1
1	A	40	TYR	HB2	2.48	0.029	1
1	A	40	TYR	HD1	6.57	0.100	1
1	A	40	TYR	HE1	6.71	0.100	1
1	A	40	TYR	C	175.01	0.143	1
1	A	41	THR	N	116.38	0.076	1
1	A	41	THR	H	9.13	0.020	1
1	A	41	THR	CA	58.58	0.160	1
1	A	41	THR	HA	5.35	0.030	1
1	A	41	THR	CB	71.81	0.159	1
1	A	41	THR	HB	3.9	0.029	1
1	A	41	THR	CG2	18.75	0.232	1
1	A	41	THR	HG21	1.01	0.030	1
1	A	41	THR	HG22	1.01	0.030	1
1	A	41	THR	HG23	1.01	0.030	1
1	A	41	THR	C	172.88	0.143	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	42	CYS	N	126.92	0.076	1
1	A	42	CYS	H	7.5	0.020	1
1	A	42	CYS	CA	55.76	0.245	1
1	A	42	CYS	HA	4.47	0.053	1
1	A	42	CYS	CB	31.48	0.198	1
1	A	42	CYS	HB2	2.6	0.067	1
1	A	42	CYS	HB3	3.33	0.051	1
1	A	43	PRO	CA	64.87	0.162	1
1	A	43	PRO	HA	4.32	0.033	1
1	A	43	PRO	CB	32.6	0.211	1
1	A	43	PRO	HB2	2.4	0.036	1
1	A	43	PRO	HB3	1.93	0.040	1
1	A	43	PRO	CG	27.72	0.181	1
1	A	43	PRO	HG2	2.17	0.051	1
1	A	43	PRO	HG3	2.01	0.049	1
1	A	43	PRO	CD	51.64	0.218	1
1	A	43	PRO	HD3	3.98	0.040	1
1	A	43	PRO	HD2	4.33	0.036	1
1	A	43	PRO	C	177.7	0.143	1
1	A	44	MET	N	117.61	0.077	1
1	A	44	MET	H	9.25	0.020	1
1	A	44	MET	CA	55.16	0.169	1
1	A	44	MET	HA	4.48	0.040	1
1	A	44	MET	CB	32.95	0.164	1
1	A	44	MET	HB2	1.64	0.036	1
1	A	44	MET	CG	32.96	0.239	1
1	A	44	MET	HG2	2.58	0.037	1
1	A	44	MET	CE	17.23	0.243	1
1	A	44	MET	HE1	2.28	0.040	1
1	A	44	MET	HE2	2.28	0.040	1
1	A	44	MET	HE3	2.28	0.040	1
1	A	44	MET	C	175.82	0.143	1
1	A	45	HIS	N	119.65	0.072	1
1	A	45	HIS	H	7.63	0.020	1
1	A	45	HIS	CA	56.61	0.189	1
1	A	45	HIS	HA	5.18	0.032	1
1	A	45	HIS	CB	32.3	0.204	1
1	A	45	HIS	HB2	3.17	0.053	1
1	A	45	HIS	HB3	3.17	0.040	1
1	A	45	HIS	HD2	7.37	0.100	1
1	A	46	PRO	CA	63.86	0.161	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	46	PRO	HA	4.73	0.029	1
1	A	46	PRO	CB	31.78	0.166	1
1	A	46	PRO	HB2	1.98	0.043	1
1	A	46	PRO	HB3	2.38	0.034	1
1	A	46	PRO	CG	27.21	0.243	1
1	A	46	PRO	HG2	1.99	0.062	1
1	A	46	PRO	HG3	1.98	0.033	1
1	A	46	PRO	CD	50.66	0.180	1
1	A	46	PRO	HD3	3.33	0.034	1
1	A	46	PRO	HD2	3.81	0.037	1
1	A	46	PRO	C	177.14	0.143	1
1	A	47	GLU	N	116.52	0.072	1
1	A	47	GLU	H	9.27	0.020	1
1	A	47	GLU	CA	57.2	0.163	1
1	A	47	GLU	HA	4.32	0.027	1
1	A	47	GLU	CB	27.44	0.160	1
1	A	47	GLU	HB2	2.17	0.107	1
1	A	47	GLU	HB3	2.17	0.038	1
1	A	47	GLU	CG	33.91	0.239	1
1	A	47	GLU	HG2	2.57	0.037	1
1	A	47	GLU	HG3	2.16	0.076	1
1	A	47	GLU	C	177.12	0.143	1
1	A	48	ILE	N	124.65	0.077	1
1	A	48	ILE	H	8.4	0.020	1
1	A	48	ILE	CA	58.77	0.160	1
1	A	48	ILE	HA	4.24	0.031	1
1	A	48	ILE	CB	34.76	0.164	1
1	A	48	ILE	HB	2.65	0.038	1
1	A	48	ILE	CG1	26.41	0.218	1
1	A	48	ILE	HG12	1.76	0.033	1
1	A	48	ILE	HG13	2.11	0.029	1
1	A	48	ILE	CG2	17.05	0.214	1
1	A	48	ILE	HG21	1.05	0.029	1
1	A	48	ILE	HG22	1.05	0.029	1
1	A	48	ILE	HG23	1.05	0.029	1
1	A	48	ILE	CD1	8.53	0.183	1
1	A	48	ILE	HD11	0.78	0.040	1
1	A	48	ILE	HD12	0.78	0.040	1
1	A	48	ILE	HD13	0.78	0.040	1
1	A	48	ILE	C	174.68	0.143	1
1	A	49	ARG	N	128.16	0.077	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	49	ARG	H	8.53	0.020	1
1	A	49	ARG	CA	54.82	0.159	1
1	A	49	ARG	HA	5.04	0.043	1
1	A	49	ARG	CB	33.6	0.162	1
1	A	49	ARG	HB2	1.68	0.039	1
1	A	49	ARG	CG	27.5	0.308	1
1	A	49	ARG	HG2	1.65	0.047	1
1	A	49	ARG	CD	43.69	0.228	1
1	A	49	ARG	HD2	3.2	0.033	1
1	A	49	ARG	C	175.38	0.143	1
1	A	50	GLN	N	120.24	0.077	1
1	A	50	GLN	H	9.34	0.020	1
1	A	50	GLN	CA	54.49	0.160	1
1	A	50	GLN	HA	5.06	0.038	1
1	A	50	GLN	CB	32.05	0.222	1
1	A	50	GLN	HB2	2.45	0.041	1
1	A	50	GLN	CG	33.39	0.332	1
1	A	50	GLN	HG2	2.45	0.059	1
1	A	50	GLN	C	176.0	0.143	1
1	A	51	SER	N	114.64	0.072	1
1	A	51	SER	H	8.95	0.020	1
1	A	51	SER	CA	59.54	0.160	1
1	A	51	SER	HA	4.86	0.025	1
1	A	51	SER	CB	64.18	0.160	1
1	A	51	SER	HB2	4.08	0.033	1
1	A	51	SER	C	173.19	0.143	1
1	A	52	ALA	N	124.26	0.072	1
1	A	52	ALA	H	7.47	0.020	1
1	A	52	ALA	CA	49.69	0.188	1
1	A	52	ALA	HA	4.67	0.029	1
1	A	52	ALA	CB	20.3	0.188	1
1	A	52	ALA	HB1	1.26	0.030	1
1	A	52	ALA	HB2	1.26	0.030	1
1	A	52	ALA	HB3	1.26	0.030	1
1	A	53	PRO	CA	61.84	0.159	1
1	A	53	PRO	HA	3.3	0.032	1
1	A	53	PRO	CB	32.03	0.162	1
1	A	53	PRO	HB2	1.88	0.036	1
1	A	53	PRO	HB3	1.56	0.029	1
1	A	53	PRO	CG	26.83	0.190	1
1	A	53	PRO	HG2	1.92	0.046	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	53	PRO	HG3	1.78	0.049	1
1	A	53	PRO	CD	49.82	0.175	1
1	A	53	PRO	HD3	3.32	0.039	1
1	A	53	PRO	HD2	3.28	0.083	1
1	A	54	GLY	N	105.42	0.090	1
1	A	54	GLY	H	7.88	0.030	1
1	A	54	GLY	CA	45.57	0.162	1
1	A	54	GLY	HA2	3.82	0.042	1
1	A	54	GLY	HA3	4.16	0.038	1
1	A	54	GLY	C	172.1	0.143	1
1	A	55	HIS	N	119.16	0.077	1
1	A	55	HIS	H	8.97	0.020	1
1	A	55	HIS	CA	54.34	0.163	1
1	A	55	HIS	HA	5.19	0.041	1
1	A	55	HIS	CB	31.68	0.187	1
1	A	55	HIS	HB2	2.87	0.039	1
1	A	55	HIS	HD2	7.37	0.100	1
1	A	45	HIS	HE1	7.83	0.100	1
1	A	55	HIS	HE1	7.83	0.100	1
1	A	55	HIS	C	173.01	0.143	1
1	A	56	CYS	N	125.76	0.077	1
1	A	56	CYS	H	9.59	0.020	1
1	A	56	CYS	CA	58.06	0.216	1
1	A	56	CYS	HA	4.48	0.054	1
1	A	56	CYS	CB	31.62	0.192	1
1	A	56	CYS	HB2	3.36	0.051	1
1	A	56	CYS	HB3	2.96	0.054	1
1	A	57	PRO	CA	64.65	0.160	1
1	A	57	PRO	HA	4.52	0.039	1
1	A	57	PRO	CB	32.24	0.169	1
1	A	57	PRO	HB2	2.44	0.044	1
1	A	57	PRO	HB3	2.05	0.033	1
1	A	57	PRO	CG	27.42	0.181	1
1	A	57	PRO	HG2	2.17	0.072	1
1	A	57	PRO	HG3	2.07	0.035	1
1	A	57	PRO	CD	51.53	0.216	1
1	A	57	PRO	HD3	3.98	0.039	1
1	A	57	PRO	HD2	4.37	0.057	1
1	A	57	PRO	C	176.57	0.143	1
1	A	58	LEU	N	122.07	0.077	1
1	A	58	LEU	H	9.44	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	58	LEU	CA	56.82	0.160	1
1	A	58	LEU	HA	4.35	0.029	1
1	A	58	LEU	CB	41.32	0.162	1
1	A	58	LEU	HB2	1.05	0.100	1
1	A	58	LEU	HB3	0.9	0.100	1
1	A	58	LEU	CG	26.8	0.250	1
1	A	58	LEU	HG	1.37	0.100	1
1	A	58	LEU	CD2	22.28	0.176	1
1	A	58	LEU	CD1	25.5	0.200	1
1	A	58	LEU	HD21	0.67	0.036	1
1	A	58	LEU	HD22	0.67	0.036	1
1	A	58	LEU	HD23	0.67	0.036	1
1	A	58	LEU	HD11	0.53	0.089	1
1	A	58	LEU	HD12	0.53	0.089	1
1	A	58	LEU	HD13	0.53	0.089	1
1	A	58	LEU	C	178.62	0.143	1
1	A	59	CYS	N	116.9	0.077	1
1	A	59	CYS	H	8.35	0.020	1
1	A	59	CYS	CA	58.6	0.161	1
1	A	59	CYS	HA	5.18	0.036	1
1	A	59	CYS	CB	34.4	0.187	1
1	A	59	CYS	C	176.98	0.143	1
1	A	60	GLY	N	112.95	0.077	1
1	A	60	GLY	H	8.31	0.020	1
1	A	60	GLY	CA	46.44	0.162	1
1	A	60	GLY	HA3	4.34	0.036	1
1	A	60	GLY	HA2	3.82	0.036	1
1	A	60	GLY	C	174.1	0.143	1
1	A	61	MET	N	123.59	0.077	1
1	A	61	MET	H	8.65	0.020	1
1	A	61	MET	CA	57.85	0.170	1
1	A	61	MET	HA	4.38	0.030	1
1	A	61	MET	CB	33.67	0.163	1
1	A	61	MET	HB2	2.47	0.036	1
1	A	61	MET	HB3	2.2	0.030	1
1	A	61	MET	CG	33.8	0.232	1
1	A	61	MET	HG2	2.96	0.029	1
1	A	61	MET	HG3	2.75	0.029	1
1	A	61	MET	CE	17.24	0.216	1
1	A	61	MET	HE1	2.19	0.030	1
1	A	61	MET	HE2	2.19	0.030	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	61	MET	HE3	2.19	0.030	1
1	A	61	MET	C	176.27	0.143	1
1	A	62	ALA	N	124.26	0.076	1
1	A	62	ALA	H	8.87	0.020	1
1	A	62	ALA	CA	53.31	0.242	1
1	A	62	ALA	HA	4.03	0.030	1
1	A	62	ALA	CB	18.07	0.166	1
1	A	62	ALA	HB1	1.37	0.029	1
1	A	62	ALA	HB2	1.37	0.029	1
1	A	62	ALA	HB3	1.37	0.029	1
1	A	62	ALA	C	177.29	0.143	1
1	A	63	LEU	N	119.16	0.077	1
1	A	63	LEU	H	8.17	0.020	1
1	A	63	LEU	CA	53.92	0.161	1
1	A	63	LEU	HA	4.54	0.028	1
1	A	63	LEU	CB	42.53	0.161	1
1	A	63	LEU	HB2	1.4	0.100	1
1	A	63	LEU	HB3	1.56	0.039	1
1	A	63	LEU	CG	26.8	0.250	1
1	A	63	LEU	HG	1.2	0.100	1
1	A	63	LEU	CD2	22.3	0.300	1
1	A	63	LEU	CD1	25.5	0.300	1
1	A	63	LEU	HD21	0.6	0.100	1
1	A	63	LEU	HD22	0.6	0.100	1
1	A	63	LEU	HD23	0.6	0.100	1
1	A	63	LEU	HD11	0.54	0.100	1
1	A	63	LEU	HD12	0.54	0.100	1
1	A	63	LEU	HD13	0.54	0.100	1
1	A	63	LEU	C	177.7	0.143	1
1	A	64	GLU	N	120.14	0.076	1
1	A	64	GLU	H	9.75	0.020	1
1	A	64	GLU	CA	52.14	0.187	1
1	A	64	GLU	HA	5.2	0.035	1
1	A	64	GLU	CB	30.11	0.200	1
1	A	64	GLU	HB2	2.09	0.075	1
1	A	64	GLU	HB3	2.48	0.048	1
1	A	64	GLU	CG	33.22	0.458	1
1	A	64	GLU	HG2	2.15	0.058	1
1	A	64	GLU	HG3	1.92	0.052	1
1	A	65	PRO	CA	62.37	0.160	1
1	A	65	PRO	HA	4.22	0.038	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	65	PRO	CB	32.07	0.166	1
1	A	65	PRO	HB2	1.9	0.075	1
1	A	65	PRO	HB3	1.67	0.048	1
1	A	65	PRO	CG	27.3	0.288	1
1	A	65	PRO	HG2	1.67	0.036	1
1	A	65	PRO	HG3	2.06	0.059	1
1	A	65	PRO	CD	50.68	0.182	1
1	A	65	PRO	HD3	3.33	0.038	1
1	A	65	PRO	HD2	3.83	0.040	1
1	A	65	PRO	C	177.26	0.143	1
1	A	66	GLU	N	122.48	0.076	1
1	A	66	GLU	H	9.01	0.020	1
1	A	66	GLU	CA	55.5	0.166	1
1	A	66	GLU	HA	4.38	0.041	1
1	A	66	GLU	CB	30.25	0.209	1
1	A	66	GLU	HB2	1.88	0.033	1
1	A	66	GLU	CG	33.09	0.182	1
1	A	66	GLU	HG2	2.31	0.033	1
1	A	66	GLU	C	175.56	0.143	1
1	A	67	THR	N	117.0	0.072	1
1	A	67	THR	H	8.51	0.020	1
1	A	67	THR	CA	62.39	0.170	1
1	A	67	THR	HA	4.5	0.047	1
1	A	67	THR	CB	69.94	0.167	1
1	A	67	THR	HB	4.41	0.079	1
1	A	67	THR	CG2	21.79	0.241	1
1	A	67	THR	HG21	1.17	0.033	1
1	A	67	THR	HG22	1.17	0.033	1
1	A	67	THR	HG23	1.17	0.033	1
1	A	67	THR	C	174.7	0.143	1
1	A	68	VAL	N	123.18	0.072	1
1	A	68	VAL	H	8.42	0.020	1
1	A	68	VAL	CA	56.55	0.214	1
1	A	68	VAL	HA	4.21	0.039	1
1	A	68	VAL	CB	32.92	0.188	1
1	A	68	VAL	HB	2.03	0.049	1
1	A	68	VAL	CG1	21.07	0.193	1
1	A	68	VAL	HG11	0.87	0.050	1
1	A	68	VAL	HG12	0.87	0.050	1
1	A	68	VAL	HG13	0.87	0.050	1
1	A	68	VAL	CG2	21.1	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	68	VAL	HG21	0.88	0.037	1
1	A	68	VAL	HG22	0.88	0.037	1
1	A	68	VAL	HG23	0.88	0.037	1
1	A	68	VAL	C	176.18	0.143	1
1	A	69	THR	N	118.86	0.072	1
1	A	69	THR	H	8.38	0.020	1
1	A	69	THR	CA	62.3	0.172	1
1	A	69	THR	HA	4.39	0.035	1
1	A	69	THR	CB	70.05	0.168	1
1	A	69	THR	HB	4.11	0.056	1
1	A	69	THR	CG2	21.73	0.243	1
1	A	69	THR	HG21	1.19	0.035	1
1	A	69	THR	HG22	1.19	0.035	1
1	A	69	THR	HG23	1.19	0.035	1
1	A	69	THR	C	174.46	0.143	1
1	A	70	VAL	N	123.64	0.071	1
1	A	70	VAL	H	8.45	0.020	1
1	A	70	VAL	CA	62.45	0.169	1
1	A	70	VAL	HA	4.18	0.028	1
1	A	70	VAL	CB	32.9	0.166	1
1	A	70	VAL	HB	2.07	0.026	1
1	A	70	VAL	CG1	20.85	0.191	1
1	A	70	VAL	CG2	20.85	0.191	1
1	A	70	VAL	HG11	0.94	0.029	1
1	A	70	VAL	HG12	0.94	0.029	1
1	A	70	VAL	HG13	0.94	0.029	1
1	A	70	VAL	HG21	0.94	0.036	1
1	A	70	VAL	HG22	0.94	0.036	1
1	A	70	VAL	HG23	0.94	0.036	1
1	A	70	VAL	C	176.23	0.143	1
1	A	71	SER	N	119.33	0.072	1
1	A	71	SER	H	8.52	0.020	1
1	A	71	SER	CA	58.74	0.236	1
1	A	71	SER	HA	4.51	0.038	1
1	A	71	SER	CB	64.16	0.187	1
1	A	71	SER	HB2	3.85	0.038	1
1	A	71	SER	C	174.51	0.143	1
1	A	72	GLU	N	122.67	0.072	1
1	A	72	GLU	H	8.5	0.020	1
1	A	72	GLU	CA	55.95	0.197	1
1	A	72	GLU	HA	4.39	0.037	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	72	GLU	CB	29.29	0.176	1
1	A	72	GLU	HB2	2.0	0.029	1
1	A	72	GLU	CG	33.62	0.216	1
1	A	72	GLU	HG2	2.38	0.041	1
1	A	72	GLU	C	176.02	0.143	1
1	A	73	VAL	N	122.04	0.072	1
1	A	73	VAL	H	8.27	0.030	1
1	A	73	VAL	CA	62.58	0.183	1
1	A	73	VAL	HA	4.08	0.029	1
1	A	73	VAL	CB	32.63	0.161	1
1	A	73	VAL	HB	2.03	0.030	1
1	A	73	VAL	CG1	20.97	0.186	1
1	A	73	VAL	HG11	0.93	0.029	1
1	A	73	VAL	HG12	0.93	0.029	1
1	A	73	VAL	HG13	0.93	0.029	1
1	A	73	VAL	HG21	0.93	0.035	1
1	A	73	VAL	HG22	0.93	0.035	1
1	A	73	VAL	HG23	0.93	0.035	1
1	A	73	VAL	C	176.25	0.143	1
1	A	74	VAL	N	124.94	0.072	1
1	A	74	VAL	H	8.44	0.020	1
1	A	74	VAL	CA	62.31	0.165	1
1	A	74	VAL	HA	4.16	0.028	1
1	A	74	VAL	CB	32.73	0.200	1
1	A	74	VAL	HB	2.05	0.030	1
1	A	74	VAL	CG1	20.94	0.193	1
1	A	74	VAL	HG11	0.92	0.030	1
1	A	74	VAL	HG12	0.92	0.030	1
1	A	74	VAL	HG13	0.92	0.030	1
1	A	74	VAL	HG21	0.91	0.036	1
1	A	74	VAL	HG22	0.91	0.036	1
1	A	74	VAL	HG23	0.91	0.036	1
1	A	74	VAL	C	175.95	0.143	1
1	A	75	SER	N	121.72	0.072	1
1	A	75	SER	H	8.62	0.020	1
1	A	75	SER	CA	56.61	0.192	1
1	A	75	SER	HA	4.79	0.029	1
1	A	75	SER	CB	63.44	0.194	1
1	A	75	SER	HB2	3.89	0.030	1
1	A	76	PRO	CA	63.73	0.166	1
1	A	76	PRO	HA	4.42	0.031	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	76	PRO	CB	32.1	0.165	1
1	A	76	PRO	HB2	2.3	0.030	1
1	A	76	PRO	CG	27.47	0.191	1
1	A	76	PRO	HG2	2.02	0.034	1
1	A	76	PRO	CD	50.8	0.186	1
1	A	76	PRO	HD2	3.82	0.031	1
1	A	76	PRO	C	177.19	0.143	1
1	A	77	GLU	N	119.37	0.072	1
1	A	77	GLU	H	8.47	0.020	1
1	A	77	GLU	CA	56.77	0.161	1
1	A	77	GLU	HA	4.23	0.025	1
1	A	77	GLU	CB	28.96	0.163	1
1	A	77	GLU	HB2	1.96	0.025	1
1	A	77	GLU	CG	33.77	0.186	1
1	A	77	GLU	HG2	2.3	0.025	1
1	A	77	GLU	C	176.39	0.143	1
1	A	78	TYR	N	120.21	0.072	1
1	A	78	TYR	H	8.17	0.020	1
1	A	78	TYR	CA	58.55	0.183	1
1	A	78	TYR	HA	4.56	0.025	1
1	A	78	TYR	CB	38.65	0.159	1
1	A	78	TYR	HB2	3.05	0.027	1
1	A	78	TYR	C	176.13	0.143	1
1	A	79	LEU	N	122.79	0.072	1
1	A	79	LEU	H	8.1	0.020	1
1	A	79	LEU	CA	55.63	0.162	1
1	A	79	LEU	HA	4.24	0.025	1
1	A	79	LEU	CB	42.4	0.160	1
1	A	79	LEU	HB2	1.57	0.028	1
1	A	79	LEU	CG	26.88	0.190	1
1	A	79	LEU	HG	1.54	0.029	1
1	A	79	LEU	CD1	24.78	0.209	1
1	A	79	LEU	CD2	23.6	0.300	1
1	A	79	LEU	HD11	0.89	0.030	1
1	A	79	LEU	HD12	0.89	0.030	1
1	A	79	LEU	HD13	0.89	0.030	1
1	A	79	LEU	HD21	0.87	0.039	1
1	A	79	LEU	HD22	0.87	0.039	1
1	A	79	LEU	HD23	0.87	0.039	1
1	A	79	LEU	C	177.11	0.143	1
1	A	80	ASP	N	119.61	0.071	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	80	ASP	H	8.35	0.020	1
1	A	80	ASP	CA	53.92	0.165	1
1	A	80	ASP	HA	4.59	0.025	1
1	A	80	ASP	CB	39.58	0.160	1
1	A	80	ASP	HB2	2.81	0.028	1
1	A	80	ASP	C	176.24	0.143	1
1	A	81	MET	N	120.82	0.072	1
1	A	81	MET	H	8.37	0.020	1
1	A	81	MET	CA	55.75	0.176	1
1	A	81	MET	HA	4.46	0.030	1
1	A	81	MET	CB	39.55	0.240	1
1	A	81	MET	HB2	2.1	0.032	1
1	A	81	MET	CG	31.98	0.187	1
1	A	81	MET	HG2	2.57	0.028	1
1	A	81	MET	CE	17.08	0.256	1
1	A	81	MET	HE1	2.1	0.031	1
1	A	81	MET	HE2	2.1	0.031	1
1	A	81	MET	HE3	2.1	0.031	1
1	A	81	MET	C	176.67	0.143	1
1	A	82	ARG	N	120.9	0.072	1
1	A	82	ARG	H	8.27	0.020	1
1	A	82	ARG	CA	56.34	0.178	1
1	A	82	ARG	HA	4.3	0.028	1
1	A	82	ARG	CB	30.5	0.184	1
1	A	82	ARG	HB2	1.86	0.026	1
1	A	82	ARG	CG	27.04	0.191	1
1	A	82	ARG	HG2	1.64	0.032	1
1	A	82	ARG	CD	43.4	0.187	1
1	A	82	ARG	HD2	3.19	0.030	1
1	A	82	ARG	C	176.43	0.143	1
1	A	83	ARG	N	122.23	0.072	1
1	A	83	ARG	H	8.39	0.020	1
1	A	83	ARG	CA	56.25	0.178	1
1	A	83	ARG	HA	4.34	0.028	1
1	A	83	ARG	CB	30.69	0.183	1
1	A	83	ARG	HB2	1.84	0.028	1
1	A	83	ARG	CG	27.05	0.191	1
1	A	83	ARG	HG2	1.67	0.039	1
1	A	83	ARG	CD	43.36	0.188	1
1	A	83	ARG	HD2	3.2	0.029	1
1	A	83	ARG	C	175.7	0.143	1

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
$^{13}\text{C}_\alpha$	83	0.96 ± 1.03	None needed (imprecise)
$^{13}\text{C}_\beta$	76	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	74	1.22 ± 1.39	None needed (imprecise)
^{15}N	74	-1.18 ± 1.76	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 4%, i.e. 16 atoms were assigned a chemical shift out of a possible 384. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	10/142 (7%)	4/57 (7%)	4/60 (7%)	2/25 (8%)
Sidechain	6/217 (3%)	4/144 (3%)	2/69 (3%)	0/4 (0%)
Aromatic	0/25 (0%)	0/12 (0%)	0/9 (0%)	0/4 (0%)
Overall	16/384 (4%)	8/213 (4%)	6/138 (4%)	2/33 (6%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 5%, i.e. 20 atoms were assigned a chemical shift out of a possible 443. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	14/166 (8%)	6/67 (9%)	6/70 (9%)	2/29 (7%)
Sidechain	6/252 (2%)	4/168 (2%)	2/80 (2%)	0/4 (0%)
Aromatic	0/25 (0%)	0/12 (0%)	0/9 (0%)	0/4 (0%)
Overall	20/443 (5%)	10/247 (4%)	8/159 (5%)	2/37 (5%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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:

