W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB NMR Structure Validation Summary Report (i)

Jun 17, 2024 – 02:16 AM EDT

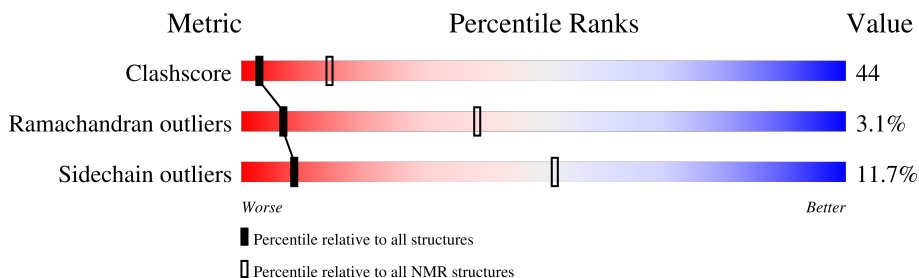|		
PDB ID	:	5OAY
BMRB ID	:	34153
Title	:	M. tuberculosis [4Fe-4S] protein WhiB1 is a four-helix bundle that forms a NO-sensitive complex with sigmaA and regulates the major virulence factor ESX-1
Authors	:	Williamson, M.P.; Green, J.; Hounslow, A.M.
Deposited on	:	2017-06-25

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 66%.

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	Percentile Ranks	Value
Clashscore		44
Ramachandran outliers		3.1%
Sidechain outliers		11.7%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all NMR structures

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	94	43% 29% • 6% 19%

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:1-A:55, A:62-A:76 (70)	0.91	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	2, 3, 8
2	4, 9
Single-model clusters	1; 5; 6; 7; 10

3 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 1160 atoms, of which 563 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcriptional regulator WhiB1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	76	1152	361	563	111	111	6	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ALA	-	expression tag	UNP P9WF43
A	-8	GLY	-	expression tag	UNP P9WF43
A	-7	GLU	-	expression tag	UNP P9WF43
A	-6	ASN	-	expression tag	UNP P9WF43
A	-5	LEU	-	expression tag	UNP P9WF43
A	-4	TYR	-	expression tag	UNP P9WF43
A	-3	PHE	-	expression tag	UNP P9WF43
A	-2	GLN	-	expression tag	UNP P9WF43
A	-1	GLY	-	expression tag	UNP P9WF43
A	0	ALA	-	expression tag	UNP P9WF43

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).
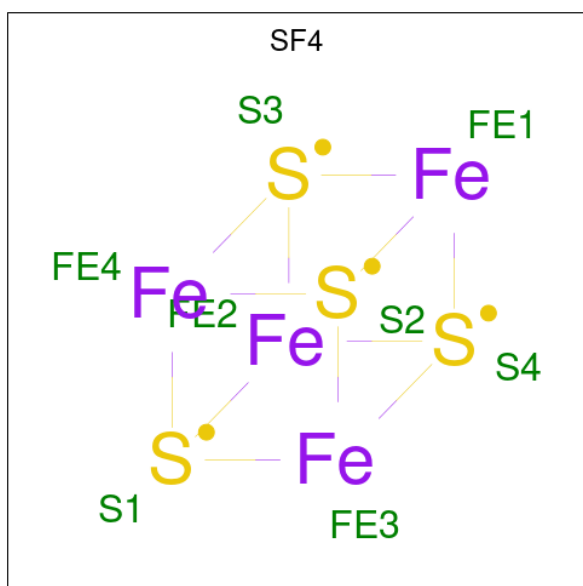
Mol	Chain	Residues	Atoms		
			Total	Fe	S
2	A	1	8	4	4

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: Transcriptional regulator WhiB1
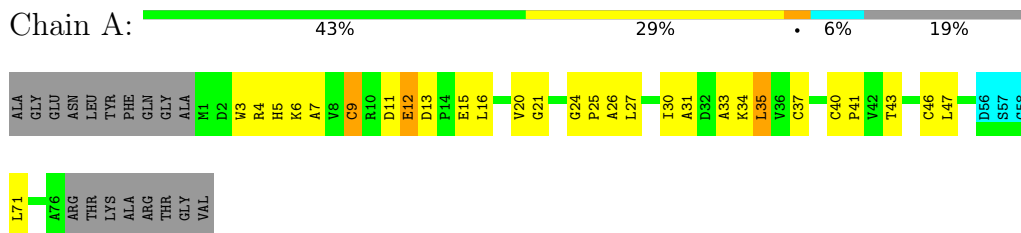
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 4. Colouring as in section 4.1 above.

• Molecule 1: Transcriptional regulator WhiB1
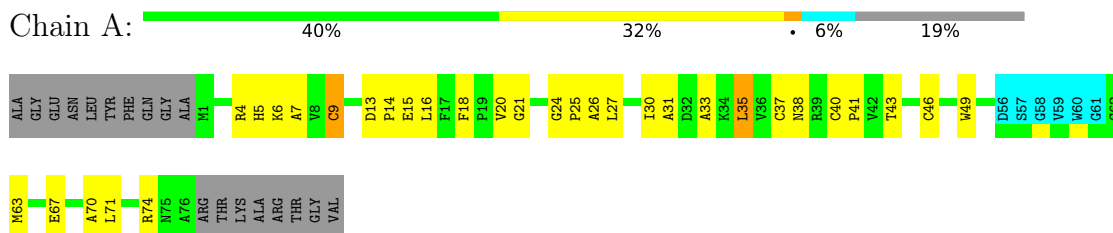
5 Refinement protocol and experimental data overview ⓘ

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

Of the 62 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
CNS	structure calculation	1.2

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	859
Number of shifts mapped to atoms	676
Number of unparsed shifts	0
Number of shifts with mapping errors	183
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	66%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	546	529	530	48±4
2	A	8	0	0	3±1
All	All	5540	5290	5300	477

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 44.

5 of 139 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:16:LEU:HD22	1:A:30:ILE:HG23	1.01	1.32	6	9
1:A:16:LEU:CD2	1:A:30:ILE:HG23	1.00	1.86	10	9
1:A:16:LEU:HD11	1:A:30:ILE:HG23	0.98	1.33	4	1
1:A:16:LEU:CD1	1:A:30:ILE:HG23	0.90	1.95	4	1
1:A:37:CYS:O	2:A:101:SF4:S3	0.90	2.29	1	6

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	68/94 (72%)	64±1 (94±1%)	2±1 (3±1%)	2±1 (3±1%)	7	39
All	All	680/940 (72%)	636 (94%)	23 (3%)	21 (3%)	7	39

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	21	GLY	8
1	A	12	GLU	6
1	A	41	PRO	4
1	A	42	VAL	2
1	A	62	GLY	1

6.3.2 Protein sidechains ⓘ

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	58/74 (78%)	51±2 (88±3%)	7±2 (12±3%)	9	52
All	All	580/740 (78%)	512 (88%)	68 (12%)	9	52

5 of 22 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	40	CYS	8
1	A	46	CYS	8
1	A	9	CYS	7
1	A	11	ASP	6
1	A	35	LEU	5

6.3.3   RNA ⓘ

There are no RNA molecules in this entry.

6.4   Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6   Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	SF4	A	101	1	0,12,12	0.00±0.00	-

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	SF4	A	101	1	-	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	A	101	1	-	-	0±0,6,5,5

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SF4 A 101
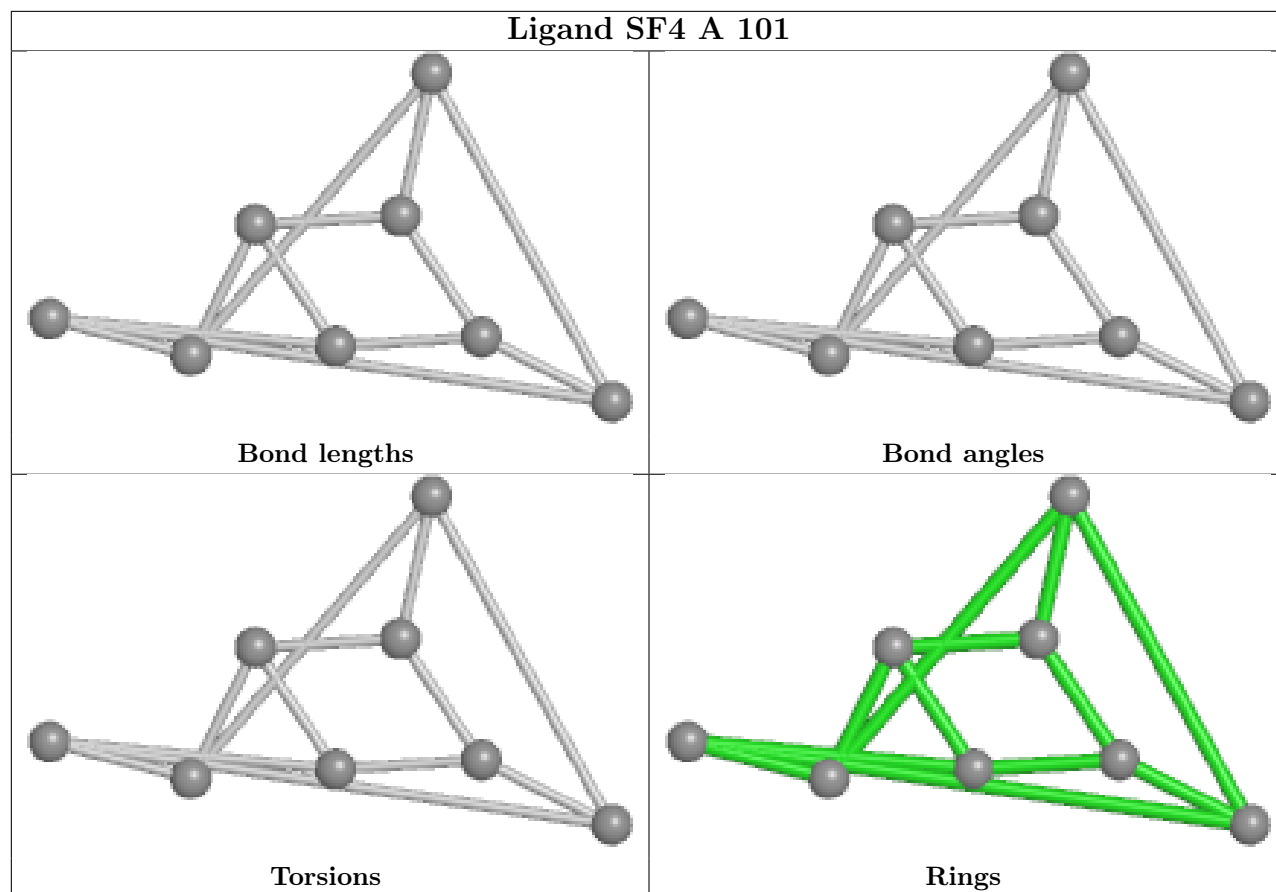
6.7 Other polymers ⓘ

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 66% for the well-defined parts and 67% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *WhiB1_new_STAR_3.1*

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	859
Number of shifts mapped to atoms	676
Number of unparsed shifts	0
Number of shifts with mapping errors	183
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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 183) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	-9	ALA	N	123.531	0.050	1
1	A	-9	ALA	H	7.88	0.005	1
1	A	-9	ALA	C	179.362	0.050	1
1	A	-9	ALA	CA	52.661	0.050	1
1	A	-9	ALA	HA	4.33	0.005	1
1	A	-9	ALA	CB	19.087	0.050	1
1	A	-9	ALA	HB1	1.55	0.005	1
1	A	-9	ALA	HB2	1.55	0.005	1
1	A	-9	ALA	HB3	1.55	0.005	1
1	A	-8	GLY	N	105.109	0.050	1
1	A	-8	GLY	H	7.712	0.005	1
1	A	-8	GLY	C	174.294	0.050	1
1	A	-8	GLY	CA	46.39	0.050	1
1	A	-8	GLY	HA2	3.89	0.005	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	-8	GLY	HA3	3.79	0.005	2
1	A	-7	GLU	N	120.085	0.050	1
1	A	-7	GLU	H	8.385	0.005	1
1	A	-7	GLU	C	176.459	0.050	1
1	A	-7	GLU	CA	56.53	0.050	1
1	A	-7	GLU	HA	4.27	0.005	1
1	A	-6	ASN	N	119.735	0.050	1
1	A	-6	ASN	H	8.561	0.005	1
1	A	-6	ASN	C	175.023	0.050	1
1	A	-6	ASN	CA	53.552	0.050	1
1	A	-6	ASN	HA	4.47	0.005	1
1	A	-6	ASN	CB	38.214	0.050	1
1	A	-6	ASN	HB2	2.73	0.005	2
1	A	-6	ASN	HB3	2.73	0.005	2
1	A	-5	LEU	N	121.239	0.050	1
1	A	-5	LEU	H	7.9	0.005	1
1	A	-5	LEU	C	176.716	0.050	1
1	A	-5	LEU	CA	55.406	0.050	1
1	A	-5	LEU	HA	4.09	0.005	1
1	A	-5	LEU	CB	42.151	0.050	1
1	A	-5	LEU	HB2	1.15	0.005	2
1	A	-5	LEU	HB3	1.3	0.005	2
1	A	-5	LEU	CG	26.6	0.050	1
1	A	-5	LEU	HG	1.25	0.005	1
1	A	-5	LEU	CD1	23.3	0.050	2
1	A	-5	LEU	HD11	0.61	0.005	2
1	A	-5	LEU	HD12	0.61	0.005	2
1	A	-5	LEU	HD13	0.61	0.005	2
1	A	-5	LEU	CD2	24.7	0.050	2
1	A	-5	LEU	HD21	0.7	0.005	2
1	A	-5	LEU	HD22	0.7	0.005	2
1	A	-5	LEU	HD23	0.7	0.005	2
1	A	-4	TYR	N	118.927	0.050	1
1	A	-4	TYR	H	7.994	0.005	1
1	A	-4	TYR	C	175.573	0.050	1
1	A	-4	TYR	CA	57.816	0.050	1
1	A	-4	TYR	HA	4.42	0.005	1
1	A	-4	TYR	CB	38.175	0.050	1
1	A	-4	TYR	HB2	2.75	0.005	2
1	A	-4	TYR	HB3	2.9	0.005	2
1	A	-4	TYR	CD1	133.0	0.050	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	-4	TYR	CD2	133.0	0.050	1
1	A	-4	TYR	HD1	6.95	0.005	1
1	A	-4	TYR	HD2	6.95	0.005	1
1	A	-4	TYR	CE1	118.1	0.050	1
1	A	-4	TYR	CE2	118.1	0.050	1
1	A	-4	TYR	HE1	6.74	0.005	1
1	A	-4	TYR	HE2	6.74	0.005	1
1	A	-3	PHE	N	121.185	0.050	1
1	A	-3	PHE	H	7.846	0.005	1
1	A	-3	PHE	C	175.588	0.050	1
1	A	-3	PHE	CA	57.633	0.050	1
1	A	-3	PHE	HA	4.53	0.005	1
1	A	-3	PHE	CB	39.406	0.050	1
1	A	-3	PHE	HB2	2.92	0.005	2
1	A	-3	PHE	HB3	3.1	0.005	2
1	A	-3	PHE	CD1	131.7	0.050	1
1	A	-3	PHE	CD2	131.7	0.050	1
1	A	-3	PHE	HD1	7.1	0.005	1
1	A	-3	PHE	HD2	7.1	0.005	1
1	A	-2	GLN	N	121.583	0.050	1
1	A	-2	GLN	H	8.559	0.005	1
1	A	-2	GLN	C	176.193	0.050	1
1	A	-2	GLN	CA	55.901	0.050	1
1	A	-2	GLN	HA	4.56	0.005	1
1	A	-2	GLN	CB	28.849	0.050	1
1	A	-2	GLN	HB2	2.14	0.005	2
1	A	-2	GLN	HB3	1.93	0.005	2
1	A	-2	GLN	CG	33.7	0.050	1
1	A	-2	GLN	HG2	2.3	0.005	2
1	A	-2	GLN	HG3	2.3	0.005	2
1	A	-1	GLY	N	109.719	0.050	1
1	A	-1	GLY	H	8.108	0.005	1
1	A	-1	GLY	C	174.238	0.050	1
1	A	-1	GLY	CA	45.317	0.050	1
1	A	-1	GLY	HA2	3.84	0.005	2
1	A	-1	GLY	HA3	4.08	0.005	2
1	A	0	ALA	N	123.594	0.050	1
1	A	0	ALA	H	8.306	0.005	1
1	A	0	ALA	C	177.771	0.050	1
1	A	0	ALA	CA	52.95	0.050	1
1	A	0	ALA	HA	4.21	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	0	ALA	CB	18.976	0.050	1
1	A	0	ALA	HB1	1.31	0.005	1
1	A	0	ALA	HB2	1.31	0.005	1
1	A	0	ALA	HB3	1.31	0.005	1
1	A	1	MET	H1	8.287	0.005	1
1	A	77	ARG	N	119.026	0.050	1
1	A	77	ARG	H	8.075	0.005	1
1	A	77	ARG	C	177.144	0.050	1
1	A	77	ARG	CA	56.761	0.050	1
1	A	77	ARG	HA	4.32	0.005	1
1	A	77	ARG	CB	30.367	0.050	1
1	A	77	ARG	HB2	1.94	0.005	2
1	A	77	ARG	HB3	1.88	0.005	2
1	A	78	THR	N	114.814	0.050	1
1	A	78	THR	H	8.062	0.005	1
1	A	78	THR	C	174.815	0.050	1
1	A	78	THR	CA	62.486	0.050	1
1	A	78	THR	HA	4.25	0.005	1
1	A	78	THR	CB	69.579	0.050	1
1	A	78	THR	HB	4.25	0.005	1
1	A	78	THR	CG2	21.55	0.050	1
1	A	78	THR	HG21	1.19	0.005	1
1	A	78	THR	HG22	1.19	0.005	1
1	A	78	THR	HG23	1.19	0.005	1
1	A	79	LYS	N	123.629	0.050	1
1	A	79	LYS	H	8.224	0.005	1
1	A	79	LYS	C	176.461	0.050	1
1	A	79	LYS	CA	56.526	0.050	1
1	A	79	LYS	HA	4.28	0.005	1
1	A	79	LYS	CB	32.697	0.050	1
1	A	79	LYS	HB2	1.84	0.005	2
1	A	79	LYS	HB3	1.78	0.005	2
1	A	80	ALA	N	124.872	0.050	1
1	A	80	ALA	H	8.232	0.005	1
1	A	80	ALA	C	177.8	0.050	1
1	A	80	ALA	CA	52.548	0.050	1
1	A	80	ALA	HA	4.28	0.005	1
1	A	80	ALA	CB	18.99	0.050	1
1	A	80	ALA	HB1	1.41	0.005	1
1	A	80	ALA	HB2	1.41	0.005	1
1	A	80	ALA	HB3	1.41	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	81	ARG	N	120.331	0.050	1
1	A	81	ARG	H	8.327	0.005	1
1	A	81	ARG	C	176.563	0.050	1
1	A	81	ARG	CA	56.151	0.050	1
1	A	81	ARG	HA	4.39	0.005	1
1	A	81	ARG	CB	30.577	0.050	1
1	A	81	ARG	HB2	1.78	0.005	2
1	A	81	ARG	HB3	1.88	0.005	2
1	A	81	ARG	CG	27.11	0.050	1
1	A	81	ARG	HG2	1.62	0.005	2
1	A	81	ARG	HG3	1.67	0.005	2
1	A	81	ARG	CD	43.22	0.050	1
1	A	81	ARG	HD2	2.84	0.005	2
1	A	81	ARG	HD3	3.19	0.005	2
1	A	82	THR	N	114.6	0.050	1
1	A	82	THR	H	8.209	0.005	1
1	A	82	THR	C	175.058	0.050	1
1	A	82	THR	CA	61.809	0.050	1
1	A	82	THR	HA	4.39	0.005	1
1	A	82	THR	CB	69.784	0.050	1
1	A	82	THR	HB	4.25	0.005	1
1	A	82	THR	CG2	21.44	0.050	1
1	A	82	THR	HG21	1.22	0.005	1
1	A	82	THR	HG22	1.22	0.005	1
1	A	82	THR	HG23	1.22	0.005	1
1	A	83	GLY	N	111.727	0.050	1
1	A	83	GLY	H	8.442	0.005	1
1	A	83	GLY	C	173.255	0.050	1
1	A	83	GLY	CA	45.352	0.050	1
1	A	83	GLY	HA2	3.95	0.005	2
1	A	83	GLY	HA3	4.07	0.005	2
1	A	84	VAL	N	122.733	0.050	1
1	A	84	VAL	H	7.63	0.005	1
1	A	84	VAL	C	181.186	0.050	1
1	A	84	VAL	CA	63.526	0.050	1
1	A	84	VAL	HA	4.08	0.005	1
1	A	84	VAL	CB	32.81	0.050	1
1	A	84	VAL	HB	2.11	0.005	1
1	A	84	VAL	CG1	19.91	0.050	2
1	A	84	VAL	HG11	0.85	0.005	2
1	A	84	VAL	HG12	0.85	0.005	2

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
					Value	Uncertainty	Ambiguity
1	A	84	VAL	HG13	0.85	0.005	2
1	A	84	VAL	CG2	21.52	0.050	2
1	A	84	VAL	HG21	0.89	0.005	2
1	A	84	VAL	HG22	0.89	0.005	2
1	A	84	VAL	HG23	0.89	0.005	2

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	89	-0.52 ± 0.28	None needed (imprecise)
$^{13}C_\beta$	71	0.51 ± 0.11	Should be checked
$^{13}C'$	88	-0.52 ± 0.20	Should be applied
^{15}N	83	0.37 ± 0.39	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 66%, i.e. 623 atoms were assigned a chemical shift out of a possible 939. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	310/346 (90%)	119/140 (85%)	131/140 (94%)	60/66 (91%)
Sidechain	279/541 (52%)	189/348 (54%)	90/163 (55%)	0/30 (0%)
Aromatic	34/52 (65%)	17/26 (65%)	15/22 (68%)	2/4 (50%)
Overall	623/939 (66%)	325/514 (63%)	236/325 (73%)	62/100 (62%)

7.1.4 Statistically unusual chemical shifts ⓘ

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	4	ARG	HB2	3.09	$0.52 - 3.08$	5.0

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7.1.5 Random Coil Index (RCI) plots ⓘ

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: