



Full wwPDB NMR Structure Validation Report ⓘ

Apr 21, 2024 – 05:52 AM EDT

PDB ID : 2M7B
BMRB ID : 19179
Title : ORF PP_3909 from *Pseudomonas putida* KT2440 encoding a protein similar to bacteriophage lambda ea8.5
Authors : Donaldson, L.W.F.
Deposited on : 2013-04-18

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 : 4.02b-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) : 2.36.2

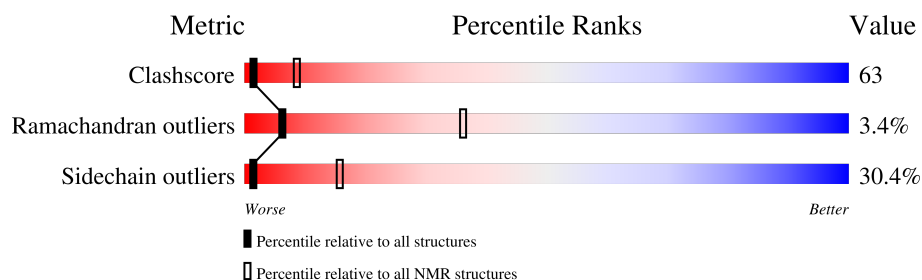
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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	94	<div> <div></div> <div>17%</div> <div>41%</div> <div>10%</div> <div>14%</div> <div>18%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:18-A:58, A:67-A:89 (64)	0.64	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 4 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1147 atoms, of which 555 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called uncharacterized protein.

Mol	Chain	Residues	Atoms						Trace
1	A	77	Total	C	H	N	O	S	0
			1146	366	555	87	134	4	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q88G17
A	0	SER	-	expression tag	UNP Q88G17

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

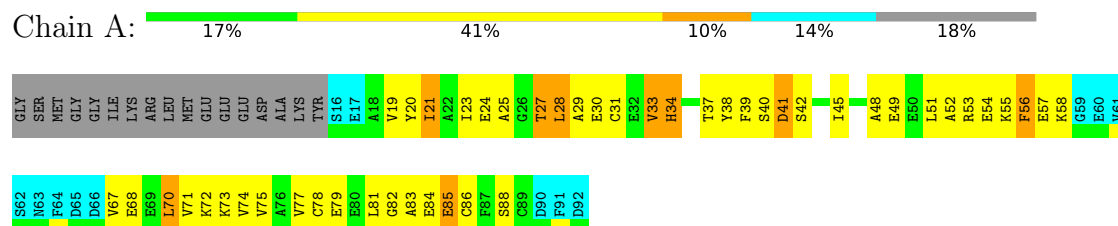
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

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: uncharacterized protein

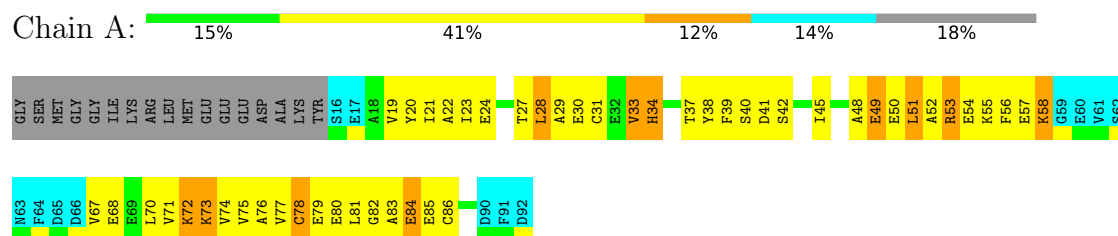


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

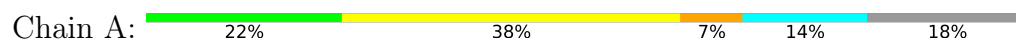
4.2.1 Score per residue for model 1 (medoid)

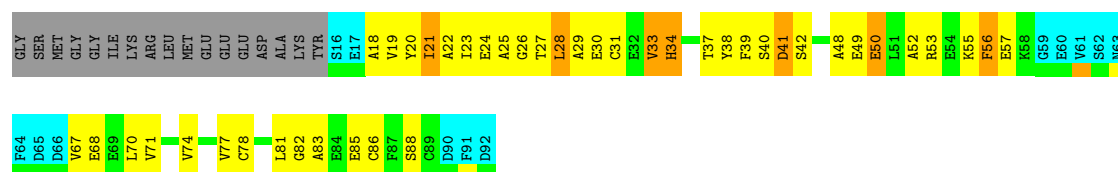
- Molecule 1: uncharacterized protein



4.2.2 Score per residue for model 2

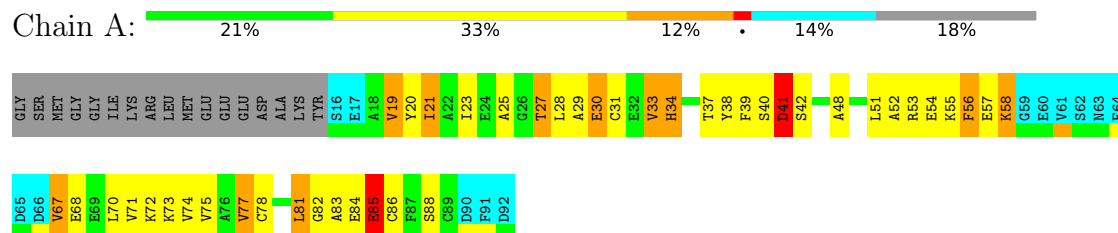
- Molecule 1: uncharacterized protein





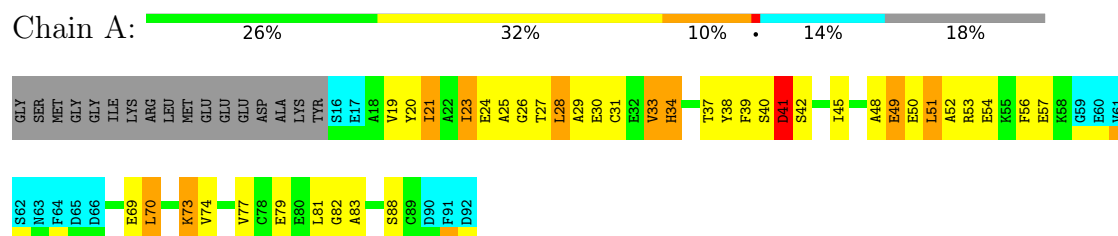
4.2.3 Score per residue for model 3

- Molecule 1: uncharacterized protein



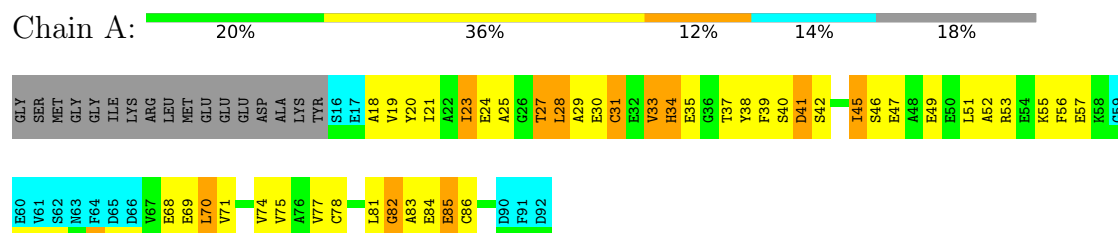
4.2.4 Score per residue for model 4

- Molecule 1: uncharacterized protein



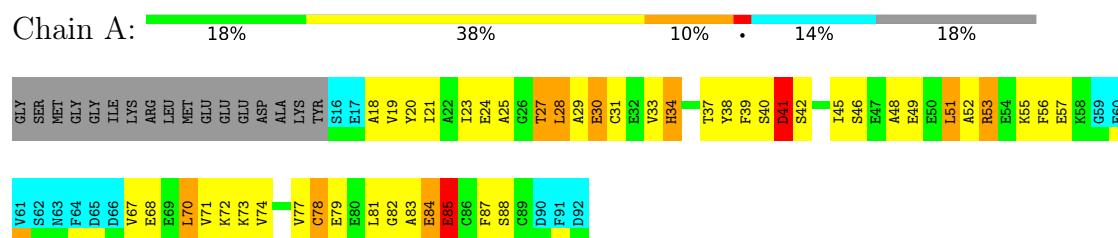
4.2.5 Score per residue for model 5

- Molecule 1: uncharacterized protein



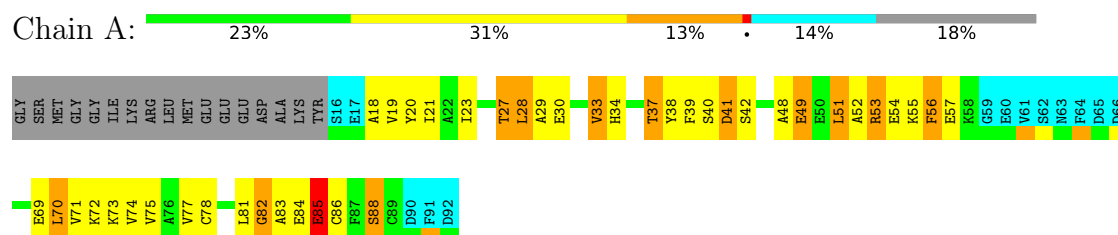
4.2.6 Score per residue for model 6

- Molecule 1: uncharacterized protein



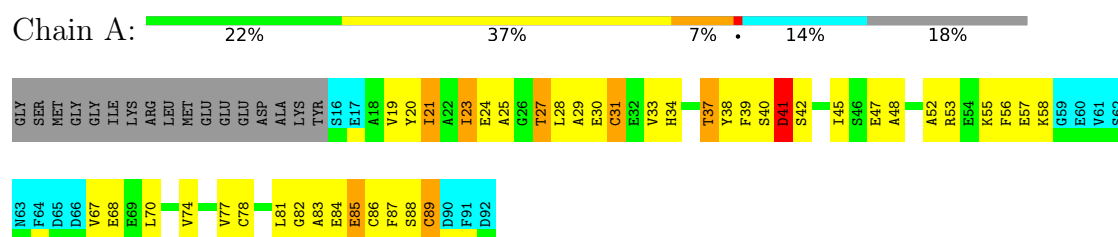
4.2.7 Score per residue for model 7

- Molecule 1: uncharacterized protein



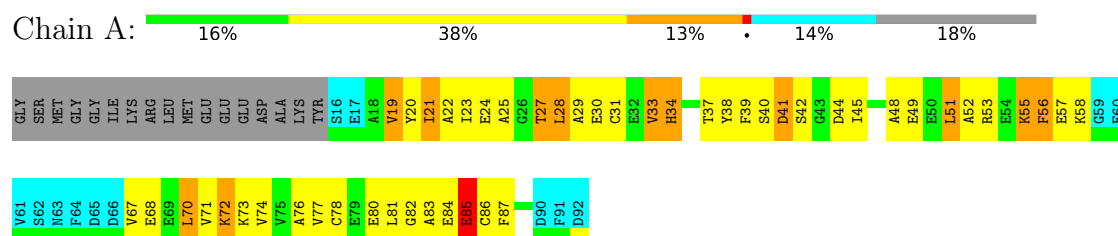
4.2.8 Score per residue for model 8

- Molecule 1: uncharacterized protein



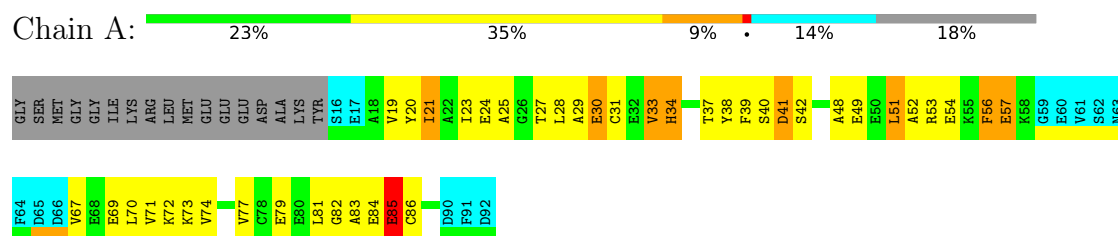
4.2.9 Score per residue for model 9

- Molecule 1: uncharacterized protein



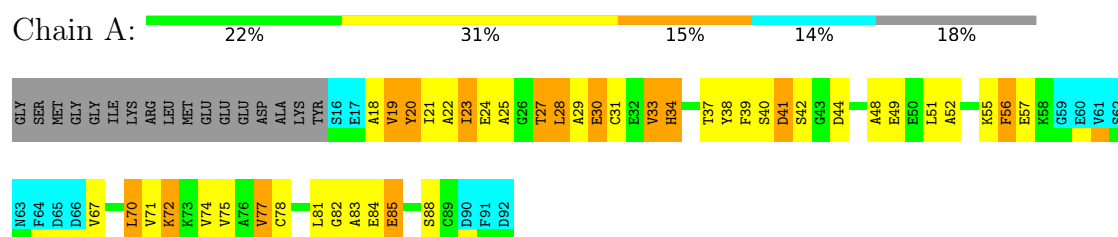
4.2.10 Score per residue for model 10

- Molecule 1: uncharacterized protein



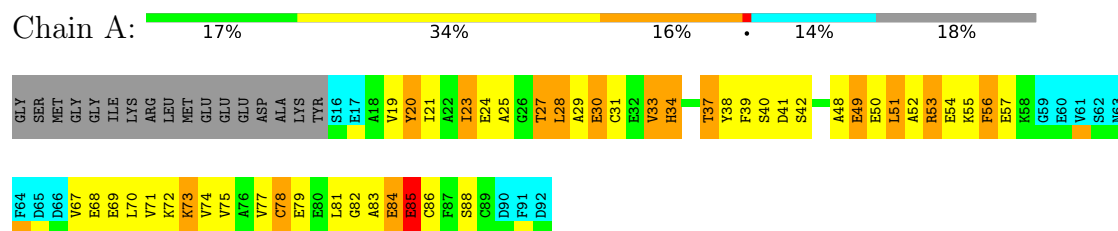
4.2.11 Score per residue for model 11

- Molecule 1: uncharacterized protein



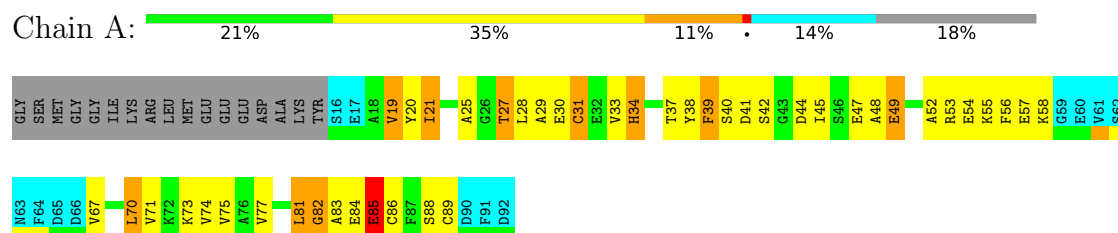
4.2.12 Score per residue for model 12

- Molecule 1: uncharacterized protein



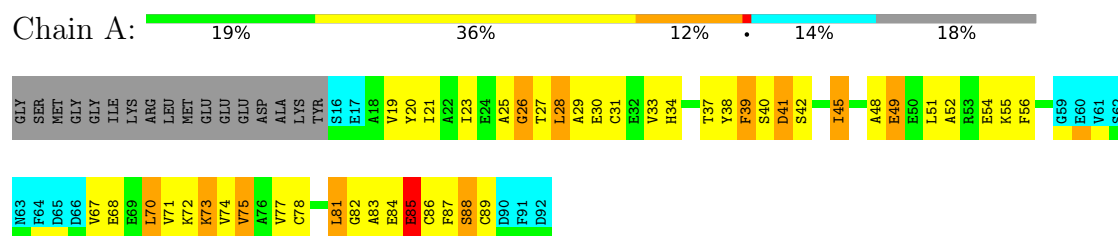
4.2.13 Score per residue for model 13

- Molecule 1: uncharacterized protein



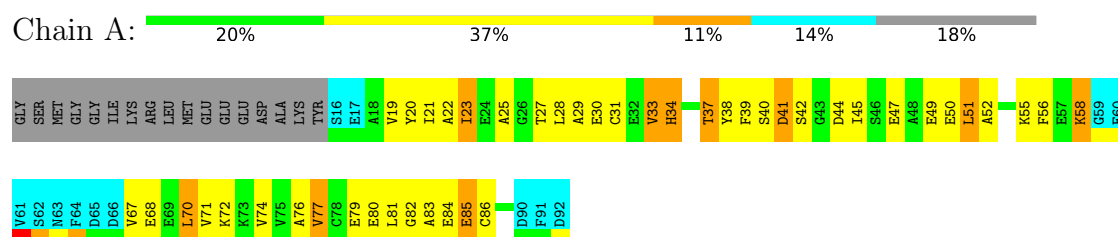
4.2.14 Score per residue for model 14

- Molecule 1: uncharacterized protein



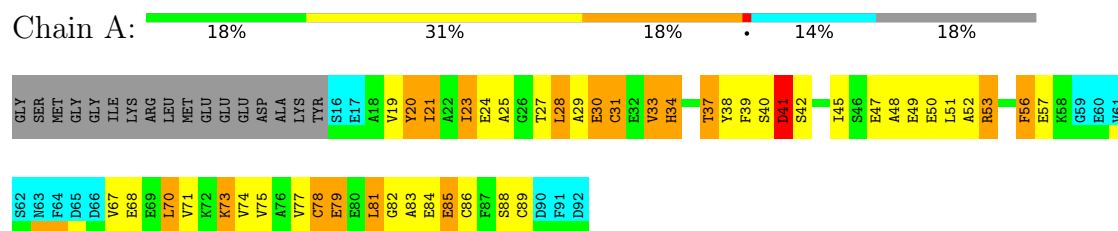
4.2.15 Score per residue for model 15

- Molecule 1: uncharacterized protein



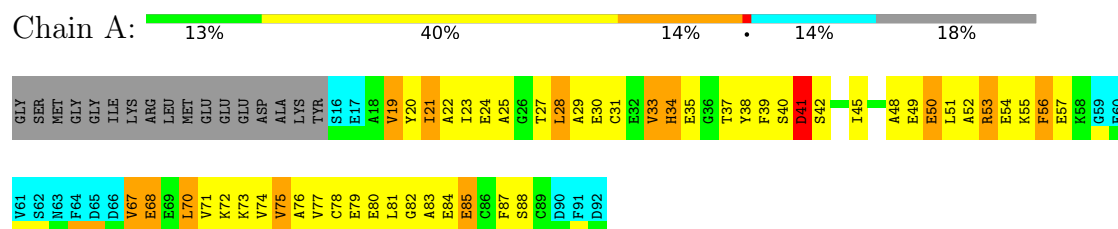
4.2.16 Score per residue for model 16

- Molecule 1: uncharacterized protein



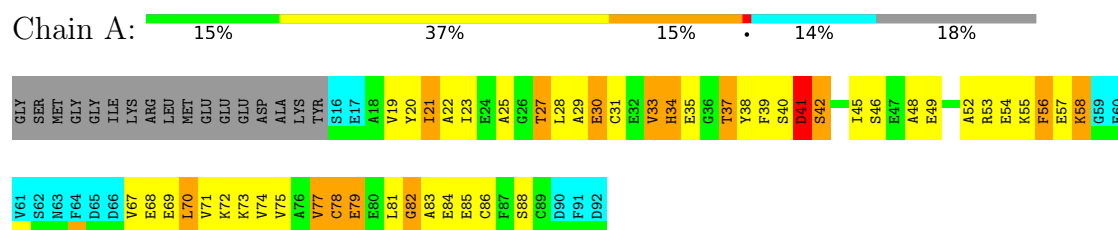
4.2.17 Score per residue for model 17

- Molecule 1: uncharacterized protein



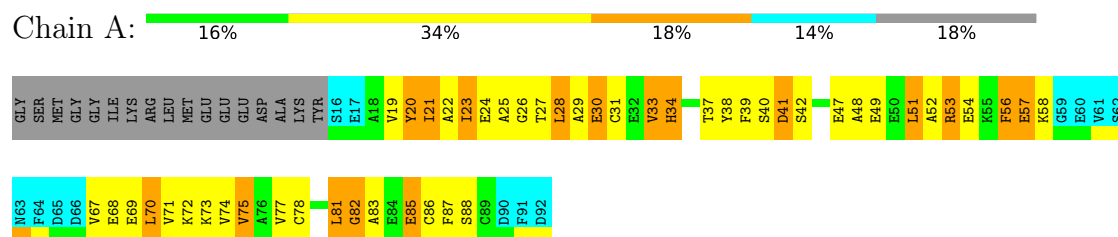
4.2.18 Score per residue for model 18

- Molecule 1: uncharacterized protein



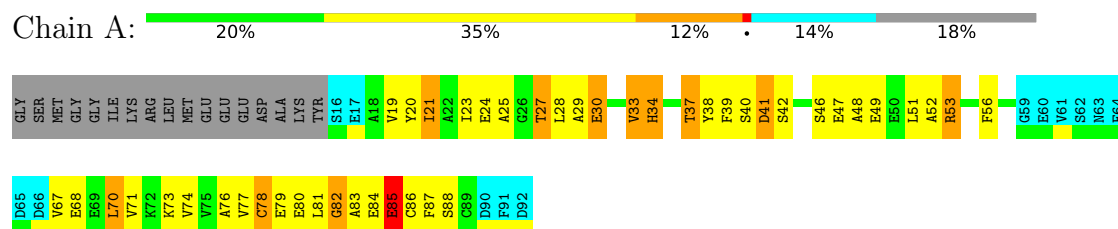
4.2.19 Score per residue for model 19

- Molecule 1: uncharacterized protein



4.2.20 Score per residue for model 20

- Molecule 1: uncharacterized protein



5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 20 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
CYANA	structure solution	3
CYANA	refinement	3

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	862
Number of shifts mapped to atoms	840
Number of unparsed shifts	0
Number of shifts with mapping errors	22
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality

6.1 Standard geometry

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

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	488	475	458	60±8
All	All	9780	9500	9160	1195

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 63.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:THR:HG23	1:A:48:ALA:HB1	1.05	1.24	12	8
1:A:23:ILE:HG22	1:A:74:VAL:HG13	1.03	1.28	20	10
1:A:51:LEU:HD23	1:A:52:ALA:N	0.98	1.73	7	1
1:A:29:ALA:HB3	1:A:39:PHE:CZ	0.97	1.94	12	20
1:A:27:THR:HG22	1:A:48:ALA:HB1	0.97	1.34	10	3
1:A:56:PHE:CD2	1:A:70:LEU:HD11	0.95	1.97	10	5
1:A:51:LEU:O	1:A:51:LEU:HD22	0.93	1.64	1	7
1:A:67:VAL:O	1:A:71:VAL:HG22	0.93	1.64	20	12
1:A:56:PHE:CE2	1:A:70:LEU:HD12	0.92	1.99	20	3
1:A:73:LYS:O	1:A:77:VAL:HG23	0.92	1.64	4	7
1:A:70:LEU:O	1:A:74:VAL:HG23	0.90	1.65	1	17
1:A:27:THR:HG22	1:A:28:LEU:HD23	0.90	1.43	19	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ILE:HG21	1:A:77:VAL:HG21	0.89	1.44	7	2
1:A:49:GLU:O	1:A:71:VAL:HG12	0.88	1.67	12	3
1:A:23:ILE:HG21	1:A:77:VAL:HG11	0.88	1.41	4	6
1:A:52:ALA:CB	1:A:74:VAL:HG21	0.88	1.97	18	4
1:A:28:LEU:HD22	1:A:40:SER:CB	0.88	1.98	10	3
1:A:27:THR:CG2	1:A:48:ALA:HB1	0.88	1.98	19	12
1:A:33:VAL:HG22	1:A:34:HIS:CE1	0.88	2.04	16	12
1:A:56:PHE:CZ	1:A:67:VAL:HG13	0.88	2.04	15	1
1:A:49:GLU:OE1	1:A:75:VAL:HG23	0.87	1.69	14	2
1:A:56:PHE:CD2	1:A:70:LEU:HD13	0.86	2.04	1	3
1:A:23:ILE:CG1	1:A:28:LEU:HD21	0.83	2.04	11	4
1:A:56:PHE:CE1	1:A:67:VAL:HG13	0.82	2.09	15	1
1:A:52:ALA:HB2	1:A:74:VAL:HG11	0.82	1.51	8	9
1:A:73:LYS:O	1:A:77:VAL:HG13	0.81	1.73	7	1
1:A:19:VAL:O	1:A:23:ILE:HG22	0.81	1.75	11	6
1:A:56:PHE:CD2	1:A:70:LEU:HD12	0.81	2.11	5	6
1:A:51:LEU:HD13	1:A:52:ALA:N	0.80	1.90	6	7
1:A:51:LEU:C	1:A:51:LEU:HD23	0.80	1.96	19	2
1:A:22:ALA:HB1	1:A:52:ALA:HB1	0.79	1.54	11	3
1:A:73:LYS:O	1:A:77:VAL:HG22	0.79	1.77	1	1
1:A:52:ALA:HB1	1:A:74:VAL:HG21	0.78	1.56	3	6
1:A:25:ALA:HB1	1:A:55:LYS:HG2	0.77	1.55	13	2
1:A:19:VAL:CG2	1:A:77:VAL:HG21	0.77	2.09	9	2
1:A:19:VAL:O	1:A:23:ILE:HG23	0.77	1.80	6	8
1:A:38:TYR:O	1:A:83:ALA:HB1	0.76	1.81	8	18
1:A:28:LEU:HD22	1:A:40:SER:HB3	0.75	1.58	16	2
1:A:52:ALA:CB	1:A:74:VAL:HG11	0.75	2.11	13	12
1:A:38:TYR:CD2	1:A:81:LEU:HD12	0.74	2.18	16	2
1:A:51:LEU:HD22	1:A:51:LEU:C	0.74	2.02	9	7
1:A:27:THR:HG21	1:A:74:VAL:CG1	0.74	2.13	17	2
1:A:56:PHE:CG	1:A:70:LEU:HD11	0.74	2.18	16	2
1:A:38:TYR:HB3	1:A:81:LEU:HD21	0.74	1.58	18	1
1:A:48:ALA:HA	1:A:51:LEU:HD12	0.73	1.61	4	2
1:A:22:ALA:HB1	1:A:52:ALA:CB	0.73	2.14	11	3
1:A:25:ALA:HB1	1:A:55:LYS:CD	0.72	2.14	9	1
1:A:56:PHE:CE2	1:A:70:LEU:CD1	0.72	2.72	6	5
1:A:23:ILE:HG22	1:A:74:VAL:CG1	0.72	2.14	6	2
1:A:56:PHE:CD2	1:A:70:LEU:HD22	0.72	2.19	2	2
1:A:52:ALA:HB3	1:A:74:VAL:HG21	0.72	1.61	2	2
1:A:56:PHE:CD2	1:A:70:LEU:CD1	0.71	2.74	18	10
1:A:56:PHE:C	1:A:56:PHE:CD1	0.70	2.65	3	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:ILE:O	1:A:25:ALA:HB2	0.70	1.87	16	5
1:A:45:ILE:HD12	1:A:78:CYS:SG	0.69	2.27	18	1
1:A:29:ALA:HB3	1:A:39:PHE:CE2	0.69	2.23	13	15
1:A:23:ILE:HG21	1:A:77:VAL:CG2	0.69	2.17	7	1
1:A:22:ALA:HB2	1:A:70:LEU:HD11	0.69	1.63	1	1
1:A:27:THR:CG2	1:A:28:LEU:HD23	0.69	2.16	19	6
1:A:51:LEU:HD13	1:A:51:LEU:C	0.69	2.08	6	1
1:A:29:ALA:CB	1:A:39:PHE:CZ	0.69	2.76	8	18
1:A:56:PHE:CE2	1:A:70:LEU:HD11	0.69	2.23	6	2
1:A:33:VAL:HG13	1:A:34:HIS:CE1	0.69	2.23	6	13
1:A:23:ILE:HG21	1:A:77:VAL:HB	0.68	1.65	17	2
1:A:27:THR:HG22	1:A:28:LEU:CD2	0.68	2.18	14	6
1:A:56:PHE:CD1	1:A:57:GLU:N	0.68	2.61	19	7
1:A:27:THR:OG1	1:A:48:ALA:HB1	0.68	1.88	7	1
1:A:33:VAL:CG2	1:A:34:HIS:CE1	0.68	2.76	17	11
1:A:23:ILE:HD12	1:A:28:LEU:HD21	0.68	1.63	15	1
1:A:27:THR:HG23	1:A:48:ALA:CB	0.67	2.18	20	10
1:A:23:ILE:HG12	1:A:77:VAL:HG11	0.67	1.65	17	2
1:A:48:ALA:O	1:A:52:ALA:HB2	0.66	1.90	4	4
1:A:51:LEU:HD23	1:A:51:LEU:C	0.66	2.11	7	2
1:A:37:THR:HG22	1:A:86:CYS:HA	0.66	1.67	7	4
1:A:38:TYR:C	1:A:83:ALA:HB1	0.66	2.11	1	17
1:A:28:LEU:HD22	1:A:78:CYS:SG	0.65	2.30	2	3
1:A:56:PHE:CZ	1:A:67:VAL:HG22	0.65	2.27	15	1
1:A:51:LEU:HD23	1:A:51:LEU:O	0.64	1.92	14	3
1:A:56:PHE:CD1	1:A:56:PHE:C	0.64	2.70	19	1
1:A:56:PHE:HD2	1:A:70:LEU:HD11	0.64	1.46	10	1
1:A:29:ALA:HB3	1:A:39:PHE:CE1	0.64	2.27	11	4
1:A:27:THR:HG23	1:A:48:ALA:CA	0.64	2.23	2	5
1:A:39:PHE:O	1:A:39:PHE:CD2	0.63	2.52	20	13
1:A:38:TYR:CD2	1:A:81:LEU:CD1	0.63	2.81	13	2
1:A:39:PHE:CD1	1:A:39:PHE:O	0.63	2.51	14	5
1:A:27:THR:HG23	1:A:28:LEU:HD12	0.63	1.69	7	1
1:A:37:THR:HG21	1:A:86:CYS:SG	0.62	2.34	16	2
1:A:56:PHE:CG	1:A:70:LEU:HD13	0.62	2.30	1	1
1:A:67:VAL:O	1:A:71:VAL:HG13	0.62	1.93	17	1
1:A:53:ARG:CG	1:A:71:VAL:HG11	0.62	2.25	5	1
1:A:39:PHE:CD1	1:A:39:PHE:C	0.62	2.73	13	2
1:A:40:SER:N	1:A:83:ALA:HB1	0.62	2.09	14	2
1:A:56:PHE:CG	1:A:70:LEU:CD1	0.61	2.83	17	3
1:A:29:ALA:O	1:A:39:PHE:CD1	0.61	2.53	18	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ILE:CG2	1:A:74:VAL:HG13	0.61	2.20	6	4
1:A:25:ALA:HB1	1:A:55:LYS:HG3	0.61	1.72	18	1
1:A:27:THR:HA	1:A:51:LEU:HD13	0.61	1.71	20	2
1:A:34:HIS:CD2	1:A:88:SER:OG	0.61	2.53	7	2
1:A:39:PHE:C	1:A:83:ALA:HB1	0.61	2.16	14	2
1:A:53:ARG:HG3	1:A:71:VAL:HG11	0.61	1.73	5	1
1:A:30:GLU:CD	1:A:38:TYR:CE1	0.60	2.75	12	1
1:A:30:GLU:CD	1:A:38:TYR:CE2	0.60	2.74	7	3
1:A:49:GLU:HB3	1:A:75:VAL:HG23	0.60	1.73	7	2
1:A:29:ALA:O	1:A:39:PHE:CD2	0.60	2.54	5	2
1:A:30:GLU:CB	1:A:38:TYR:CD2	0.60	2.84	18	8
1:A:27:THR:HG23	1:A:48:ALA:O	0.60	1.96	10	2
1:A:27:THR:CG2	1:A:28:LEU:HD12	0.60	2.27	7	1
1:A:87:PHE:CD1	1:A:88:SER:N	0.60	2.70	14	1
1:A:51:LEU:HD21	1:A:55:LYS:CE	0.60	2.27	9	1
1:A:51:LEU:C	1:A:51:LEU:CD2	0.60	2.70	19	8
1:A:30:GLU:HB3	1:A:38:TYR:CD2	0.60	2.31	18	16
1:A:39:PHE:O	1:A:39:PHE:CG	0.59	2.55	9	17
1:A:27:THR:HG23	1:A:48:ALA:HA	0.59	1.73	2	4
1:A:53:ARG:CD	1:A:53:ARG:C	0.59	2.70	12	2
1:A:85:GLU:OE1	1:A:87:PHE:CE1	0.59	2.56	19	1
1:A:27:THR:C	1:A:28:LEU:HD23	0.59	2.18	17	1
1:A:23:ILE:HG21	1:A:77:VAL:CG1	0.59	2.28	11	3
1:A:27:THR:HA	1:A:51:LEU:HD11	0.58	1.75	17	4
1:A:33:VAL:CG2	1:A:34:HIS:ND1	0.58	2.66	17	1
1:A:56:PHE:CG	1:A:57:GLU:N	0.58	2.71	19	8
1:A:23:ILE:HG22	1:A:74:VAL:HA	0.58	1.73	9	1
1:A:53:ARG:CB	1:A:71:VAL:CG1	0.58	2.81	7	4
1:A:27:THR:HG22	1:A:48:ALA:CB	0.58	2.22	10	1
1:A:48:ALA:HA	1:A:51:LEU:HD22	0.58	1.74	7	1
1:A:23:ILE:CG1	1:A:28:LEU:CD2	0.58	2.81	11	2
1:A:49:GLU:CD	1:A:75:VAL:HG23	0.57	2.18	14	1
1:A:28:LEU:HD13	1:A:40:SER:OG	0.57	1.99	10	1
1:A:28:LEU:HD22	1:A:40:SER:OG	0.57	1.98	18	3
1:A:33:VAL:HG23	1:A:34:HIS:CD2	0.57	2.34	20	1
1:A:39:PHE:CB	1:A:85:GLU:N	0.57	2.68	8	13
1:A:23:ILE:HG13	1:A:28:LEU:HD21	0.56	1.75	11	3
1:A:20:TYR:O	1:A:24:GLU:CG	0.56	2.53	10	4
1:A:84:GLU:O	1:A:85:GLU:CB	0.56	2.53	11	12
1:A:27:THR:OG1	1:A:51:LEU:HD22	0.56	2.00	19	1
1:A:19:VAL:CG2	1:A:20:TYR:N	0.56	2.68	11	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ILE:HD11	1:A:28:LEU:HD11	0.56	1.77	8	2
1:A:39:PHE:CG	1:A:39:PHE:O	0.56	2.59	16	3
1:A:34:HIS:N	1:A:34:HIS:ND1	0.55	2.54	16	12
1:A:39:PHE:CA	1:A:83:ALA:HB1	0.55	2.31	14	2
1:A:87:PHE:CG	1:A:88:SER:N	0.55	2.74	14	2
1:A:56:PHE:HZ	1:A:67:VAL:HG22	0.55	1.58	15	1
1:A:23:ILE:CD1	1:A:28:LEU:HD11	0.55	2.31	3	1
1:A:20:TYR:O	1:A:24:GLU:CB	0.55	2.54	11	12
1:A:29:ALA:HB1	1:A:39:PHE:CZ	0.55	2.37	7	2
1:A:19:VAL:HG21	1:A:73:LYS:HG2	0.55	1.79	16	1
1:A:30:GLU:OE2	1:A:38:TYR:CZ	0.55	2.59	18	1
1:A:47:GLU:CG	1:A:51:LEU:HD12	0.55	2.32	5	1
1:A:33:VAL:CG1	1:A:34:HIS:CE1	0.54	2.90	6	8
1:A:56:PHE:CE2	1:A:70:LEU:HG	0.54	2.38	14	2
1:A:53:ARG:O	1:A:57:GLU:CB	0.54	2.55	10	13
1:A:23:ILE:HG21	1:A:77:VAL:HG12	0.54	1.79	3	1
1:A:30:GLU:CG	1:A:38:TYR:CE2	0.54	2.91	8	4
1:A:26:GLY:O	1:A:51:LEU:CD1	0.54	2.56	14	1
1:A:48:ALA:O	1:A:52:ALA:CB	0.54	2.56	4	3
1:A:30:GLU:HG2	1:A:38:TYR:CD2	0.54	2.38	18	2
1:A:53:ARG:CG	1:A:54:GLU:N	0.53	2.71	19	5
1:A:53:ARG:O	1:A:56:PHE:CD2	0.53	2.61	19	1
1:A:84:GLU:O	1:A:85:GLU:CG	0.53	2.56	10	5
1:A:53:ARG:O	1:A:57:GLU:CG	0.53	2.57	17	3
1:A:30:GLU:HG3	1:A:38:TYR:CE2	0.53	2.38	8	3
1:A:48:ALA:O	1:A:74:VAL:HG11	0.53	2.04	11	1
1:A:28:LEU:HD23	1:A:78:CYS:SG	0.53	2.43	3	1
1:A:27:THR:CG2	1:A:48:ALA:CB	0.53	2.85	16	5
1:A:22:ALA:O	1:A:51:LEU:HD11	0.53	2.04	15	1
1:A:34:HIS:CE1	1:A:88:SER:HB3	0.52	2.39	17	3
1:A:27:THR:OG1	1:A:48:ALA:CB	0.52	2.56	7	1
1:A:56:PHE:CE1	1:A:67:VAL:CG1	0.52	2.88	15	1
1:A:40:SER:O	1:A:42:SER:N	0.52	2.42	19	20
1:A:23:ILE:CD1	1:A:28:LEU:HD21	0.52	2.35	11	2
1:A:29:ALA:O	1:A:39:PHE:O	0.52	2.28	18	2
1:A:52:ALA:O	1:A:56:PHE:CB	0.52	2.57	15	7
1:A:37:THR:HG21	1:A:88:SER:OG	0.52	2.05	7	1
1:A:30:GLU:HG2	1:A:38:TYR:CE2	0.52	2.40	18	2
1:A:50:GLU:CG	1:A:51:LEU:N	0.52	2.73	4	3
1:A:69:GLU:O	1:A:73:LYS:CG	0.52	2.58	12	4
1:A:27:THR:OG1	1:A:52:ALA:HB2	0.52	2.05	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:THR:CG2	1:A:86:CYS:SG	0.52	2.97	20	1
1:A:47:GLU:O	1:A:51:LEU:HD23	0.52	2.05	16	1
1:A:19:VAL:HG22	1:A:77:VAL:HG21	0.52	1.80	9	2
1:A:25:ALA:HB1	1:A:55:LYS:HD3	0.52	1.80	9	1
1:A:33:VAL:HG22	1:A:34:HIS:ND1	0.52	2.19	16	10
1:A:39:PHE:O	1:A:39:PHE:CD1	0.52	2.63	10	1
1:A:74:VAL:O	1:A:77:VAL:HG22	0.52	2.04	7	1
1:A:25:ALA:HB1	1:A:55:LYS:CG	0.52	2.32	13	1
1:A:70:LEU:O	1:A:74:VAL:N	0.51	2.42	1	2
1:A:51:LEU:O	1:A:55:LYS:CG	0.51	2.58	3	2
1:A:21:ILE:O	1:A:25:ALA:CB	0.51	2.57	16	2
1:A:26:GLY:O	1:A:51:LEU:HD13	0.51	2.06	14	1
1:A:86:CYS:SG	1:A:88:SER:OG	0.51	2.68	18	1
1:A:30:GLU:HB3	1:A:38:TYR:CD1	0.51	2.40	4	1
1:A:25:ALA:HB2	1:A:55:LYS:HD2	0.51	1.82	15	1
1:A:19:VAL:CG2	1:A:73:LYS:O	0.51	2.59	10	1
1:A:19:VAL:HG23	1:A:20:TYR:N	0.51	2.21	1	3
1:A:68:GLU:HA	1:A:71:VAL:CG2	0.51	2.36	15	8
1:A:18:ALA:O	1:A:21:ILE:HG22	0.51	2.05	11	2
1:A:23:ILE:HG12	1:A:28:LEU:HD21	0.51	1.82	4	2
1:A:34:HIS:N	1:A:34:HIS:CD2	0.51	2.79	14	2
1:A:21:ILE:O	1:A:25:ALA:N	0.51	2.43	5	15
1:A:34:HIS:CD2	1:A:88:SER:HB2	0.51	2.40	6	2
1:A:27:THR:OG1	1:A:51:LEU:CD1	0.50	2.59	1	2
1:A:27:THR:CB	1:A:48:ALA:HB1	0.50	2.36	9	1
1:A:23:ILE:HG21	1:A:77:VAL:CB	0.50	2.37	9	1
1:A:54:GLU:CG	1:A:55:LYS:N	0.50	2.74	14	1
1:A:76:ALA:O	1:A:80:GLU:CB	0.50	2.60	15	1
1:A:47:GLU:O	1:A:51:LEU:CB	0.50	2.59	20	2
1:A:58:LYS:O	1:A:58:LYS:CD	0.50	2.59	3	3
1:A:30:GLU:CG	1:A:38:TYR:CD2	0.50	2.94	18	4
1:A:56:PHE:HD2	1:A:70:LEU:HD22	0.50	1.66	1	1
1:A:78:CYS:SG	1:A:79:GLU:N	0.50	2.83	20	7
1:A:27:THR:HB	1:A:48:ALA:HB1	0.50	1.82	9	1
1:A:47:GLU:O	1:A:51:LEU:CD2	0.50	2.59	16	1
1:A:52:ALA:CB	1:A:74:VAL:CG2	0.50	2.84	18	1
1:A:27:THR:O	1:A:28:LEU:HD23	0.50	2.07	18	1
1:A:50:GLU:CD	1:A:50:GLU:C	0.50	2.70	17	1
1:A:56:PHE:CZ	1:A:57:GLU:HG2	0.50	2.42	17	1
1:A:19:VAL:HG13	1:A:20:TYR:N	0.49	2.22	5	9
1:A:27:THR:OG1	1:A:48:ALA:CA	0.49	2.60	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ALA:O	1:A:55:LYS:CE	0.49	2.59	14	1
1:A:49:GLU:OE1	1:A:75:VAL:CG2	0.49	2.60	17	1
1:A:33:VAL:HG23	1:A:34:HIS:ND1	0.49	2.23	17	1
1:A:53:ARG:O	1:A:56:PHE:CE2	0.49	2.66	19	1
1:A:53:ARG:HG3	1:A:54:GLU:N	0.49	2.22	12	1
1:A:49:GLU:OE1	1:A:75:VAL:N	0.49	2.46	19	1
1:A:19:VAL:O	1:A:23:ILE:CG2	0.49	2.59	6	3
1:A:46:SER:O	1:A:49:GLU:CG	0.49	2.61	20	4
1:A:20:TYR:O	1:A:24:GLU:N	0.48	2.46	12	6
1:A:72:LYS:O	1:A:75:VAL:HG12	0.48	2.08	1	1
1:A:53:ARG:HA	1:A:56:PHE:CD2	0.48	2.43	7	3
1:A:22:ALA:CB	1:A:70:LEU:HD21	0.48	2.39	17	1
1:A:48:ALA:O	1:A:51:LEU:CD1	0.48	2.61	4	1
1:A:56:PHE:CZ	1:A:67:VAL:CG1	0.48	2.88	15	1
1:A:68:GLU:O	1:A:72:LYS:CB	0.48	2.61	9	4
1:A:21:ILE:CG2	1:A:56:PHE:CZ	0.48	2.96	10	1
1:A:67:VAL:HG13	1:A:68:GLU:N	0.48	2.23	9	5
1:A:48:ALA:O	1:A:51:LEU:HD13	0.48	2.09	4	1
1:A:53:ARG:HA	1:A:56:PHE:CE2	0.48	2.44	7	3
1:A:53:ARG:HG2	1:A:54:GLU:N	0.48	2.24	19	1
1:A:84:GLU:O	1:A:85:GLU:HB3	0.48	2.08	13	4
1:A:19:VAL:HG21	1:A:73:LYS:O	0.48	2.09	18	1
1:A:81:LEU:O	1:A:82:GLY:C	0.48	2.52	11	20
1:A:22:ALA:O	1:A:27:THR:CG2	0.48	2.61	9	1
1:A:67:VAL:CG2	1:A:68:GLU:N	0.48	2.77	3	1
1:A:30:GLU:HB2	1:A:38:TYR:CD1	0.48	2.44	5	1
1:A:19:VAL:CG2	1:A:77:VAL:CG2	0.48	2.87	9	1
1:A:87:PHE:C	1:A:87:PHE:CD1	0.47	2.88	9	1
1:A:54:GLU:O	1:A:58:LYS:CG	0.47	2.62	19	1
1:A:27:THR:OG1	1:A:51:LEU:HD12	0.47	2.09	6	1
1:A:33:VAL:HG23	1:A:34:HIS:CE1	0.47	2.45	9	1
1:A:56:PHE:CZ	1:A:70:LEU:HG	0.47	2.44	14	1
1:A:30:GLU:OE2	1:A:38:TYR:CE2	0.47	2.68	18	1
1:A:45:ILE:HG23	1:A:78:CYS:SG	0.47	2.50	18	1
1:A:34:HIS:CG	1:A:86:CYS:SG	0.47	3.07	12	8
1:A:30:GLU:CD	1:A:38:TYR:CZ	0.47	2.87	20	2
1:A:73:LYS:O	1:A:77:VAL:CG2	0.47	2.60	14	1
1:A:30:GLU:HB3	1:A:38:TYR:CG	0.47	2.45	12	3
1:A:54:GLU:O	1:A:58:LYS:N	0.47	2.48	19	3
1:A:39:PHE:HA	1:A:83:ALA:C	0.47	2.30	14	2
1:A:70:LEU:O	1:A:70:LEU:HD22	0.47	2.09	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:GLU:O	1:A:71:VAL:HG22	0.47	2.09	14	1
1:A:45:ILE:HD13	1:A:78:CYS:SG	0.47	2.50	5	1
1:A:48:ALA:HB1	1:A:78:CYS:SG	0.47	2.49	2	1
1:A:21:ILE:CG2	1:A:56:PHE:CE2	0.47	2.97	10	1
1:A:86:CYS:SG	1:A:86:CYS:O	0.46	2.73	13	1
1:A:28:LEU:HD23	1:A:28:LEU:N	0.46	2.25	2	1
1:A:72:LYS:O	1:A:72:LYS:CE	0.46	2.64	11	1
1:A:50:GLU:HG3	1:A:51:LEU:N	0.46	2.25	17	1
1:A:56:PHE:CG	1:A:70:LEU:HD12	0.46	2.44	19	1
1:A:56:PHE:CD1	1:A:56:PHE:O	0.46	2.68	20	1
1:A:49:GLU:CG	1:A:50:GLU:N	0.46	2.78	15	4
1:A:49:GLU:CD	1:A:75:VAL:CG2	0.46	2.84	14	1
1:A:34:HIS:CD2	1:A:34:HIS:N	0.46	2.82	20	1
1:A:58:LYS:CG	1:A:58:LYS:O	0.46	2.63	9	1
1:A:30:GLU:HG2	1:A:38:TYR:CZ	0.46	2.46	5	2
1:A:19:VAL:CG1	1:A:20:TYR:N	0.46	2.79	7	2
1:A:72:LYS:O	1:A:76:ALA:CB	0.46	2.63	9	1
1:A:23:ILE:CG1	1:A:28:LEU:CD1	0.46	2.93	16	1
1:A:27:THR:HG23	1:A:51:LEU:HD11	0.46	1.87	16	1
1:A:56:PHE:CE2	1:A:67:VAL:HG23	0.46	2.46	2	1
1:A:85:GLU:N	1:A:85:GLU:OE1	0.45	2.49	15	1
1:A:49:GLU:N	1:A:49:GLU:CD	0.45	2.70	19	1
1:A:27:THR:CG2	1:A:28:LEU:N	0.45	2.78	15	1
1:A:38:TYR:CB	1:A:83:ALA:CB	0.45	2.94	4	3
1:A:23:ILE:HB	1:A:74:VAL:HG13	0.45	1.88	5	2
1:A:28:LEU:HD23	1:A:78:CYS:HB2	0.45	1.88	9	1
1:A:30:GLU:CD	1:A:30:GLU:N	0.45	2.70	4	1
1:A:56:PHE:CE2	1:A:70:LEU:CG	0.45	2.99	14	2
1:A:23:ILE:HG12	1:A:28:LEU:CD2	0.45	2.42	11	2
1:A:34:HIS:ND1	1:A:86:CYS:SG	0.45	2.89	8	2
1:A:41:ASP:CB	1:A:47:GLU:OE1	0.45	2.64	8	1
1:A:31:CYS:HB2	1:A:37:THR:CG2	0.45	2.41	16	1
1:A:48:ALA:C	1:A:74:VAL:HG11	0.45	2.32	18	1
1:A:86:CYS:O	1:A:89:CYS:N	0.45	2.49	8	1
1:A:53:ARG:HB2	1:A:71:VAL:HG11	0.45	1.87	13	1
1:A:23:ILE:HG13	1:A:28:LEU:HD11	0.45	1.87	16	1
1:A:51:LEU:HD12	1:A:52:ALA:N	0.45	2.26	17	1
1:A:28:LEU:HG	1:A:40:SER:CB	0.45	2.42	5	1
1:A:56:PHE:CZ	1:A:70:LEU:HD12	0.45	2.44	20	2
1:A:85:GLU:OE2	1:A:85:GLU:N	0.45	2.49	7	1
1:A:49:GLU:CD	1:A:50:GLU:N	0.45	2.70	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:PHE:CE2	1:A:70:LEU:CB	0.45	3.00	1	1
1:A:22:ALA:CB	1:A:52:ALA:HB1	0.45	2.37	18	1
1:A:81:LEU:O	1:A:83:ALA:N	0.45	2.50	7	6
1:A:25:ALA:O	1:A:55:LYS:NZ	0.45	2.50	17	1
1:A:71:VAL:HG23	1:A:72:LYS:N	0.44	2.28	7	3
1:A:23:ILE:HD12	1:A:77:VAL:HG11	0.44	1.87	12	1
1:A:38:TYR:CD2	1:A:81:LEU:HD13	0.44	2.47	1	1
1:A:53:ARG:O	1:A:57:GLU:N	0.44	2.50	10	3
1:A:47:GLU:CG	1:A:51:LEU:CD1	0.44	2.95	5	1
1:A:30:GLU:HG3	1:A:38:TYR:CZ	0.44	2.47	7	2
1:A:53:ARG:HB2	1:A:71:VAL:CG1	0.44	2.41	7	4
1:A:30:GLU:CD	1:A:38:TYR:CD2	0.44	2.91	8	1
1:A:38:TYR:HB2	1:A:83:ALA:CB	0.44	2.43	16	3
1:A:40:SER:CB	1:A:78:CYS:SG	0.44	3.05	19	2
1:A:20:TYR:O	1:A:24:GLU:HB2	0.44	2.13	10	4
1:A:23:ILE:CG1	1:A:28:LEU:HD11	0.44	2.42	19	2
1:A:38:TYR:CG	1:A:81:LEU:HD12	0.44	2.47	19	2
1:A:19:VAL:HG11	1:A:73:LYS:CE	0.43	2.43	1	1
1:A:34:HIS:O	1:A:37:THR:OG1	0.43	2.30	4	2
1:A:41:ASP:CB	1:A:47:GLU:CD	0.43	2.87	8	1
1:A:38:TYR:CG	1:A:81:LEU:HD22	0.43	2.48	14	1
1:A:22:ALA:HB1	1:A:70:LEU:HD21	0.43	1.90	1	1
1:A:54:GLU:O	1:A:58:LYS:CB	0.43	2.65	19	2
1:A:56:PHE:CE2	1:A:70:LEU:HD13	0.43	2.44	1	1
1:A:27:THR:OG1	1:A:48:ALA:O	0.43	2.35	3	2
1:A:76:ALA:O	1:A:80:GLU:N	0.43	2.51	1	4
1:A:30:GLU:CB	1:A:38:TYR:CD1	0.43	3.01	12	2
1:A:34:HIS:CB	1:A:37:THR:OG1	0.43	2.66	8	1
1:A:84:GLU:CG	1:A:85:GLU:N	0.43	2.81	13	1
1:A:49:GLU:OE2	1:A:74:VAL:HG12	0.43	2.13	17	1
1:A:23:ILE:O	1:A:27:THR:HG22	0.43	2.14	5	1
1:A:23:ILE:HD11	1:A:28:LEU:HD21	0.43	1.89	11	1
1:A:47:GLU:CG	1:A:51:LEU:HD23	0.43	2.43	16	1
1:A:71:VAL:O	1:A:75:VAL:HG13	0.43	2.14	18	1
1:A:30:GLU:N	1:A:30:GLU:OE1	0.43	2.51	3	2
1:A:34:HIS:CG	1:A:88:SER:HG	0.43	2.32	17	1
1:A:33:VAL:HG13	1:A:34:HIS:ND1	0.43	2.28	7	2
1:A:51:LEU:CD2	1:A:55:LYS:HG3	0.43	2.44	6	1
1:A:53:ARG:HB3	1:A:71:VAL:CG1	0.43	2.43	7	2
1:A:68:GLU:O	1:A:71:VAL:CG2	0.43	2.66	16	4
1:A:19:VAL:HG23	1:A:73:LYS:O	0.43	2.14	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ILE:HA	1:A:27:THR:CB	0.43	2.44	1	2
1:A:40:SER:N	1:A:83:ALA:CB	0.43	2.81	13	2
1:A:39:PHE:HB2	1:A:85:GLU:N	0.42	2.29	16	4
1:A:28:LEU:CB	1:A:40:SER:HA	0.42	2.44	12	3
1:A:23:ILE:CG2	1:A:77:VAL:HG11	0.42	2.43	19	1
1:A:30:GLU:CB	1:A:38:TYR:CE2	0.42	3.02	20	1
1:A:40:SER:O	1:A:41:ASP:C	0.42	2.57	7	10
1:A:39:PHE:HB3	1:A:85:GLU:N	0.42	2.29	8	5
1:A:34:HIS:CD2	1:A:88:SER:CB	0.42	3.02	6	1
1:A:25:ALA:HB2	1:A:55:LYS:HG2	0.42	1.91	8	1
1:A:53:ARG:NH2	1:A:67:VAL:HG21	0.42	2.29	10	1
1:A:20:TYR:HA	1:A:23:ILE:CG2	0.42	2.44	19	1
1:A:31:CYS:HB3	1:A:34:HIS:CG	0.42	2.49	13	1
1:A:58:LYS:O	1:A:58:LYS:CG	0.42	2.66	15	1
1:A:19:VAL:O	1:A:23:ILE:CG1	0.42	2.67	2	1
1:A:20:TYR:HA	1:A:23:ILE:CG1	0.42	2.45	3	1
1:A:18:ALA:O	1:A:22:ALA:CB	0.42	2.68	2	1
1:A:48:ALA:CA	1:A:51:LEU:HD12	0.42	2.41	4	1
1:A:35:GLU:O	1:A:35:GLU:CG	0.42	2.68	5	1
1:A:37:THR:CG2	1:A:86:CYS:HA	0.42	2.45	12	1
1:A:48:ALA:HA	1:A:51:LEU:HD21	0.42	1.90	17	1
1:A:20:TYR:HA	1:A:23:ILE:HG23	0.42	1.92	4	1
1:A:27:THR:OG1	1:A:51:LEU:HD11	0.42	2.14	4	1
1:A:44:ASP:OD2	1:A:47:GLU:N	0.42	2.53	15	1
1:A:84:GLU:O	1:A:85:GLU:HB2	0.41	2.14	1	2
1:A:72:LYS:O	1:A:76:ALA:HB2	0.41	2.15	9	1
1:A:77:VAL:CG1	1:A:78:CYS:N	0.41	2.83	11	1
1:A:56:PHE:CZ	1:A:67:VAL:HA	0.41	2.51	9	1
1:A:44:ASP:CG	1:A:47:GLU:CG	0.41	2.89	13	1
1:A:34:HIS:CB	1:A:88:SER:OG	0.41	2.69	16	1
1:A:52:ALA:O	1:A:56:PHE:HB2	0.41	2.15	13	1
1:A:84:GLU:O	1:A:85:GLU:CD	0.41	2.59	16	1
1:A:55:LYS:HE2	1:A:55:LYS:CA	0.41	2.46	17	1
1:A:28:LEU:HB3	1:A:40:SER:CB	0.41	2.46	19	1
1:A:68:GLU:CG	1:A:69:GLU:N	0.41	2.83	5	1
1:A:23:ILE:HA	1:A:27:THR:CG2	0.41	2.46	7	2
1:A:57:GLU:CG	1:A:58:LYS:N	0.41	2.84	8	1
1:A:23:ILE:CG2	1:A:74:VAL:HA	0.41	2.45	20	2
1:A:38:TYR:CB	1:A:81:LEU:HD21	0.41	2.41	18	1
1:A:70:LEU:HD13	1:A:74:VAL:CG2	0.41	2.46	8	1
1:A:70:LEU:O	1:A:74:VAL:CG2	0.41	2.59	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ILE:O	1:A:49:GLU:OE1	0.41	2.39	14	1
1:A:38:TYR:CG	1:A:81:LEU:CD1	0.41	3.03	16	2
1:A:85:GLU:CD	1:A:85:GLU:C	0.41	2.79	3	1
1:A:51:LEU:C	1:A:51:LEU:CD1	0.41	2.80	6	1
1:A:28:LEU:HD22	1:A:81:LEU:HD12	0.41	1.92	7	1
1:A:31:CYS:HB3	1:A:34:HIS:CD2	0.41	2.51	8	1
1:A:67:VAL:CG1	1:A:68:GLU:N	0.41	2.84	9	1
1:A:31:CYS:CB	1:A:37:THR:CG2	0.41	2.98	16	1
1:A:47:GLU:HG2	1:A:51:LEU:CD2	0.41	2.46	16	1
1:A:21:ILE:HG22	1:A:22:ALA:N	0.41	2.31	18	1
1:A:19:VAL:O	1:A:22:ALA:N	0.41	2.54	19	1
1:A:47:GLU:O	1:A:51:LEU:N	0.41	2.54	20	1
1:A:30:GLU:OE1	1:A:31:CYS:O	0.40	2.39	5	1
1:A:68:GLU:HA	1:A:71:VAL:HG22	0.40	1.93	6	1
1:A:30:GLU:OE1	1:A:38:TYR:CD2	0.40	2.73	7	1
1:A:84:GLU:CD	1:A:85:GLU:N	0.40	2.75	14	1
1:A:34:HIS:ND1	1:A:88:SER:OG	0.40	2.49	17	1
1:A:37:THR:CG2	1:A:88:SER:OG	0.40	2.69	4	1
1:A:20:TYR:O	1:A:23:ILE:HG13	0.40	2.15	10	1
1:A:56:PHE:CD2	1:A:70:LEU:CD2	0.40	3.00	2	1
1:A:29:ALA:C	1:A:39:PHE:CE1	0.40	2.94	18	1
1:A:23:ILE:CB	1:A:74:VAL:HG13	0.40	2.46	5	1
1:A:53:ARG:CB	1:A:71:VAL:HG11	0.40	2.46	7	1
1:A:33:VAL:CG2	1:A:33:VAL:O	0.40	2.70	10	1
1:A:31:CYS:HB3	1:A:34:HIS:ND1	0.40	2.31	13	1

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	64/94 (68%)	58±1 (91±2%)	4±1 (6±2%)	2±1 (3±1%)	6	36
All	All	1280/1880 (68%)	1159 (91%)	77 (6%)	44 (3%)	6	36

All 4 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	41	ASP	20
1	A	85	GLU	14
1	A	82	GLY	6
1	A	26	GLY	4

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	52/77 (68%)	36±3 (70±6%)	16±3 (30±6%)	1	16
All	All	1040/1540 (68%)	724 (70%)	316 (30%)	1	16

All 42 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	33	VAL	19
1	A	37	THR	19
1	A	31	CYS	18
1	A	34	HIS	17
1	A	21	ILE	16
1	A	28	LEU	15
1	A	70	LEU	14
1	A	41	ASP	13
1	A	85	GLU	12
1	A	45	ILE	11
1	A	56	PHE	11
1	A	27	THR	11
1	A	51	LEU	9
1	A	53	ARG	9
1	A	77	VAL	9
1	A	30	GLU	9
1	A	49	GLU	8
1	A	73	LYS	8
1	A	75	VAL	8
1	A	23	ILE	8
1	A	72	LYS	7
1	A	78	CYS	7

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Mol	Chain	Res	Type	Models (Total)
1	A	55	LYS	5
1	A	19	VAL	5
1	A	81	LEU	5
1	A	79	GLU	5
1	A	58	LYS	4
1	A	84	GLU	4
1	A	88	SER	4
1	A	89	CYS	4
1	A	20	TYR	4
1	A	50	GLU	3
1	A	67	VAL	2
1	A	44	ASP	2
1	A	57	GLU	2
1	A	39	PHE	2
1	A	35	GLU	2
1	A	54	GLU	1
1	A	68	GLU	1
1	A	42	SER	1
1	A	69	GLU	1
1	A	24	GLU	1

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 ⓘ

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

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 88% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	862
Number of shifts mapped to atoms	840
Number of unparsed shifts	0
Number of shifts with mapping errors	22
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

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

- No matching atom found in the structure. All 22 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	14	LYS	H	7.986	.	1
1	A	14	LYS	N	118.085	.	1
1	A	13	ALA	C	180.627	.	1
1	A	15	TYR	CE1	118.442	.	3
1	A	15	TYR	CE2	118.442	.	3
1	A	4	ILE	HD11	0.892	.	1
1	A	4	ILE	HD12	0.892	.	1
1	A	4	ILE	HD13	0.892	.	1
1	A	4	ILE	CD1	12.994	.	1
1	A	4	ILE	CG2	17.729	.	1
1	A	4	ILE	HG21	0.936	.	1
1	A	4	ILE	HG22	0.936	.	1
1	A	4	ILE	HG23	0.936	.	1
1	A	15	TYR	HD1	7.154	.	3

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	15	TYR	HD2	7.154	.	3
1	A	15	TYR	CB	38.333	.	1
1	A	15	TYR	HE1	6.859	.	3
1	A	15	TYR	HE2	6.859	.	3
1	A	15	TYR	CD1	133.258	.	3
1	A	15	TYR	CD2	133.258	.	3
1	A	4	ILE	CG1	27.236	.	1
1	A	4	ILE	CB	38.833	.	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	74	-0.60 ± 0.18	Should be checked
$^{13}\text{C}_\beta$	70	0.31 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	75	-0.21 ± 0.13	None needed (< 0.5 ppm)
^{15}N	74	-0.14 ± 0.36	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 91%, i.e. 734 atoms were assigned a chemical shift out of a possible 809. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	317/324 (98%)	129/132 (98%)	125/128 (98%)	63/64 (98%)
Sidechain	376/430 (87%)	259/279 (93%)	117/144 (81%)	0/7 (0%)
Aromatic	41/55 (75%)	23/27 (85%)	18/27 (67%)	0/1 (0%)
Overall	734/809 (91%)	411/438 (94%)	260/299 (87%)	63/72 (88%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 840 atoms were assigned a chemical shift out of a possible 954. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	371/390 (95%)	150/159 (94%)	148/154 (96%)	73/77 (95%)
Sidechain	416/489 (85%)	286/314 (91%)	129/167 (77%)	1/8 (12%)
Aromatic	53/75 (71%)	31/37 (84%)	22/37 (59%)	0/1 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Overall	840/954 (88%)	467/510 (92%)	299/358 (84%)	74/86 (86%)

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	27	THR	CB	51.73	61.12 – 78.27	-10.5
1	A	43	GLY	N	130.57	91.59 – 127.52	5.8
1	A	88	SER	HB2	2.43	2.61 – 5.13	-5.7
1	A	59	GLY	N	130.07	91.59 – 127.52	5.7
1	A	26	GLY	N	129.92	91.59 – 127.52	5.7
1	A	62	SER	H	11.40	5.45 – 11.10	5.5
1	A	82	GLY	N	128.00	91.59 – 127.52	5.1

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:

