Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 06:00 PM EDT

PDB ID	:	2MN6
BMRB ID	:	19714
Title	:	Solution structure of dimeric TatA of twin-arginine translocation system from E. coli
Authors	:	Zhang, Y.; Hu, Y.; Jin, C.
Deposited on	:	2014-03-31

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 (i) 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 (i)) were used in the production of this report:

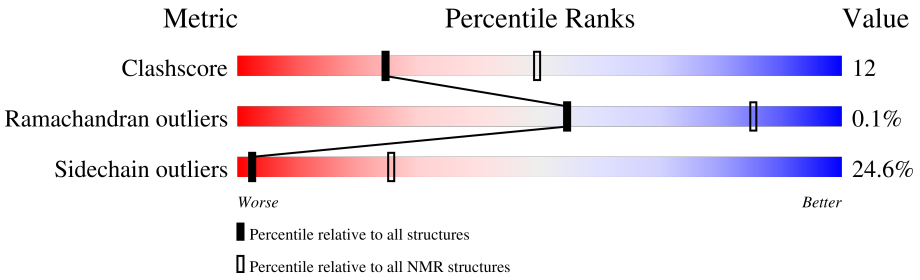
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 49%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	100	26% 13% • 7% 53%
1	B	100	25% 11% • 8% 53%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 9 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	B:6-B:44, A:6-A:45 (79)	0.59	9

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. No single-model clusters were found.

Cluster number	Models
1	1, 5, 7, 8, 9, 10
2	2, 3, 4, 6

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1438 atoms, of which 750 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sec-independent protein translocase protein TatA.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	B	47	719	226	375	54	62	2	0
1	A	47	719	226	375	54	62	2	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	expression tag	UNP P69428
B	-1	CYS	-	expression tag	UNP P69428
B	0	GLY	-	expression tag	UNP P69428
B	90	LEU	-	expression tag	UNP P69428
B	91	GLU	-	expression tag	UNP P69428
B	92	HIS	-	expression tag	UNP P69428
B	93	HIS	-	expression tag	UNP P69428
B	94	HIS	-	expression tag	UNP P69428
B	95	HIS	-	expression tag	UNP P69428
B	96	HIS	-	expression tag	UNP P69428
B	97	HIS	-	expression tag	UNP P69428
A	-2	MET	-	expression tag	UNP P69428
A	-1	CYS	-	expression tag	UNP P69428
A	0	GLY	-	expression tag	UNP P69428
A	90	LEU	-	expression tag	UNP P69428
A	91	GLU	-	expression tag	UNP P69428
A	92	HIS	-	expression tag	UNP P69428
A	93	HIS	-	expression tag	UNP P69428
A	94	HIS	-	expression tag	UNP P69428
A	95	HIS	-	expression tag	UNP P69428
A	96	HIS	-	expression tag	UNP P69428
A	97	HIS	-	expression tag	UNP P69428

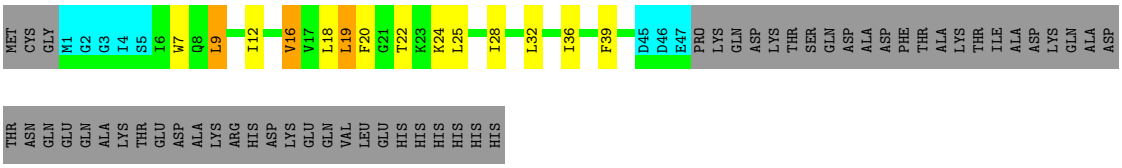
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

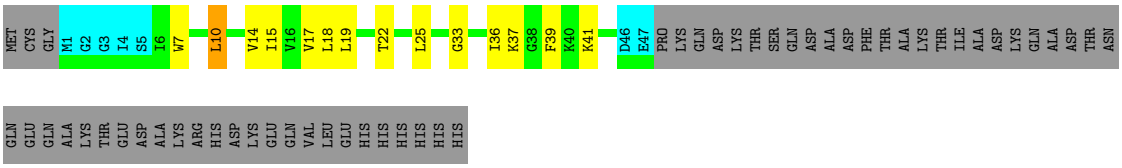
• Molecule 1: Sec-independent protein translocase protein TatA

Chain B: 25% 11% • 8% 53%



• Molecule 1: Sec-independent protein translocase protein TatA

Chain A: 26% 13% • 7% 53%



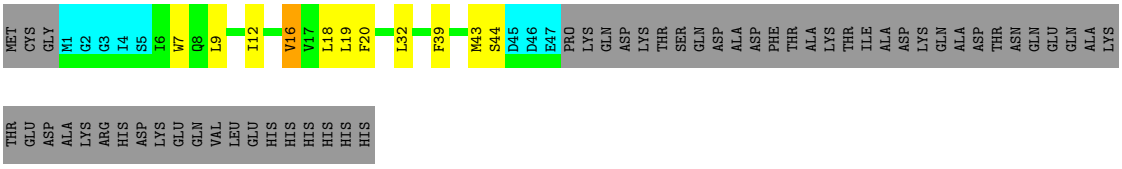
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

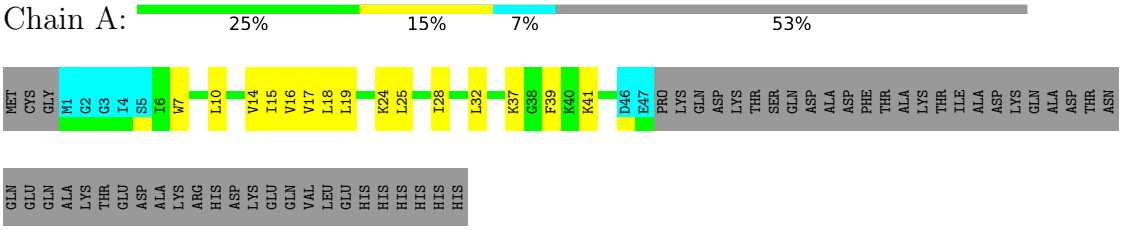
• Molecule 1: Sec-independent protein translocase protein TatA

Chain B: 28% 10% • 8% 53%



• Molecule 1: Sec-independent protein translocase protein TatA

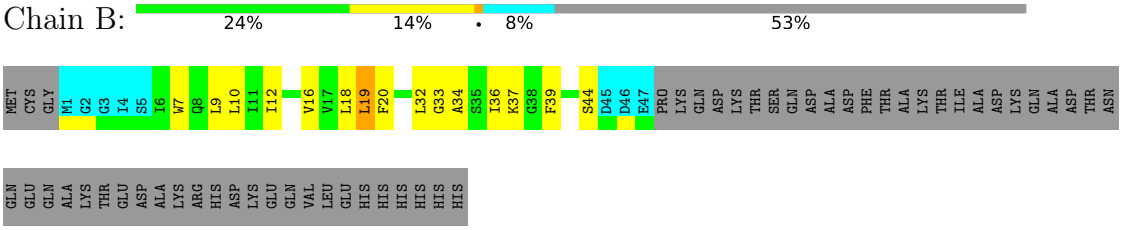
Chain A:



4.2.2 Score per residue for model 2

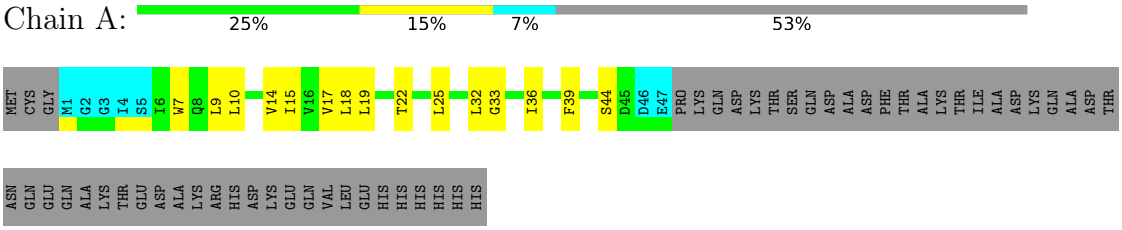
• Molecule 1: Sec-independent protein translocase protein TatA

Chain B:



• Molecule 1: Sec-independent protein translocase protein TatA

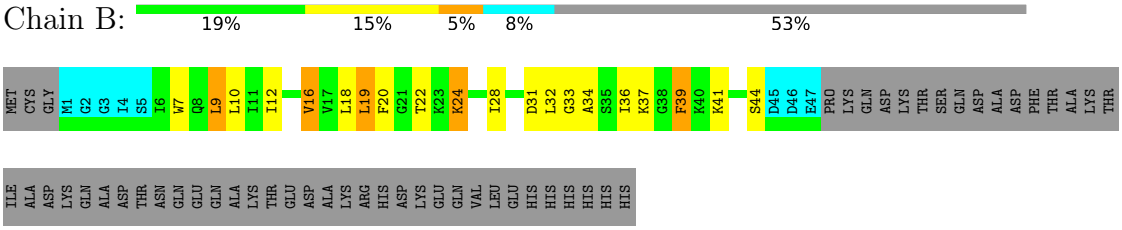
Chain A:



4.2.3 Score per residue for model 3

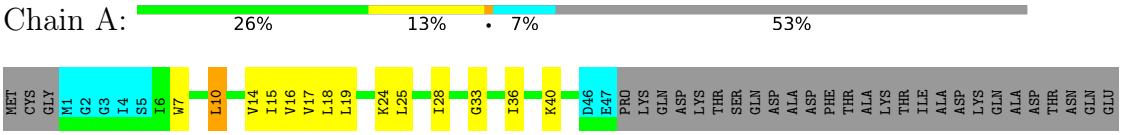
• Molecule 1: Sec-independent protein translocase protein TatA

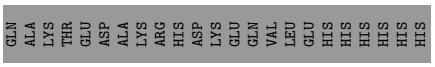
Chain B:



• Molecule 1: Sec-independent protein translocase protein TatA

Chain A:

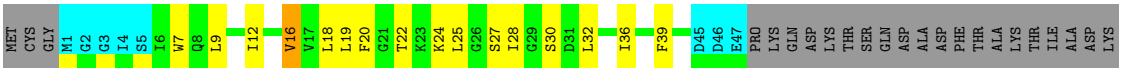




4.2.4 Score per residue for model 4

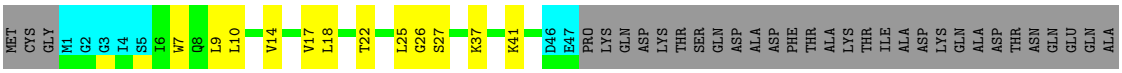
- Molecule 1: Sec-independent protein translocase protein TatA

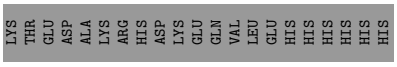
Chain B:



- Molecule 1: Sec-independent protein translocase protein TatA

Chain A:

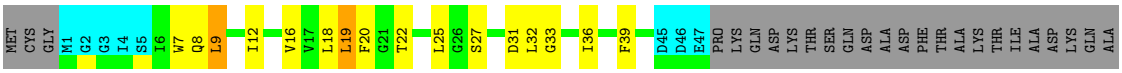




4.2.5 Score per residue for model 5

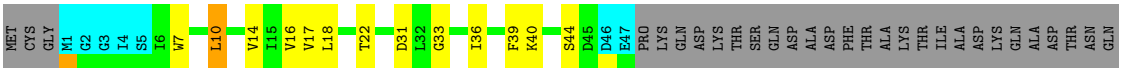
- Molecule 1: Sec-independent protein translocase protein TatA

Chain B:



- Molecule 1: Sec-independent protein translocase protein TatA

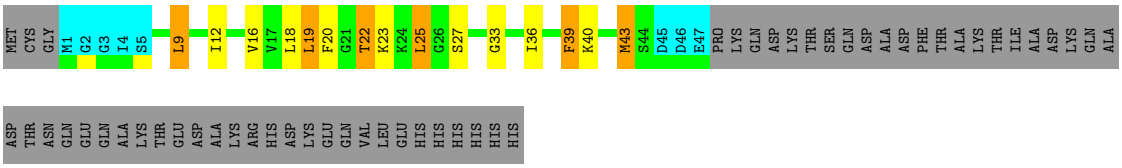
Chain A:



4.2.6 Score per residue for model 6

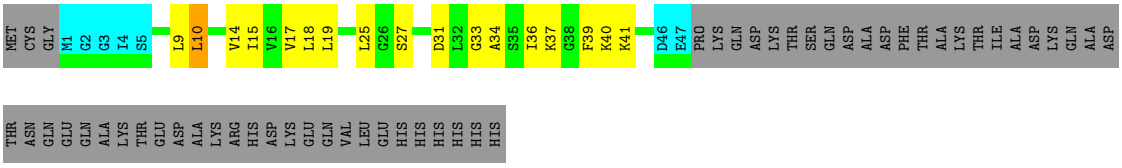
- Molecule 1: Sec-independent protein translocase protein TatA

Chain B: 24% 9% 6% 8% 53%



- Molecule 1: Sec-independent protein translocase protein TatA

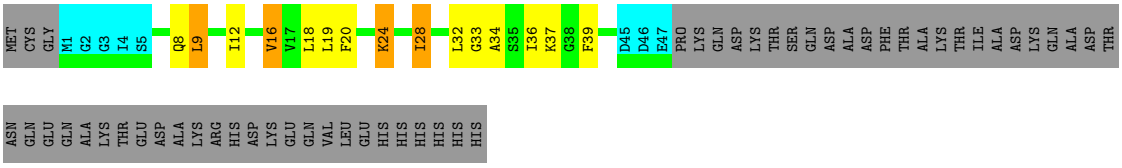
Chain A: 23% 16% • 7% 53%



4.2.7 Score per residue for model 7

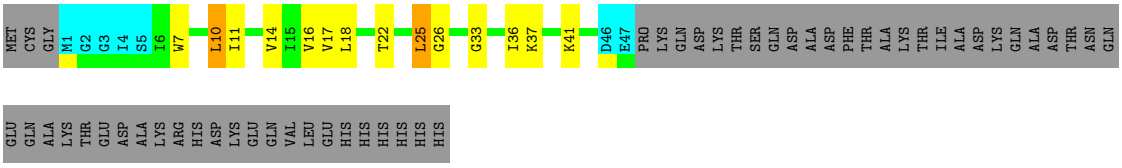
- Molecule 1: Sec-independent protein translocase protein TatA

Chain B: 24% 11% • 8% 53%



- Molecule 1: Sec-independent protein translocase protein TatA

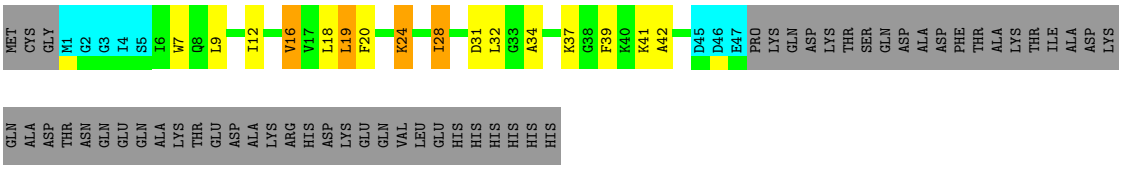
Chain A: 26% 12% • 7% 53%



4.2.8 Score per residue for model 8

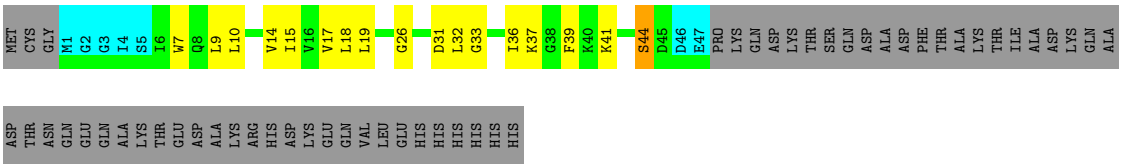
- Molecule 1: Sec-independent protein translocase protein TatA

Chain B: 23% 12% • 8% 53%



• Molecule 1: Sec-independent protein translocase protein TatA

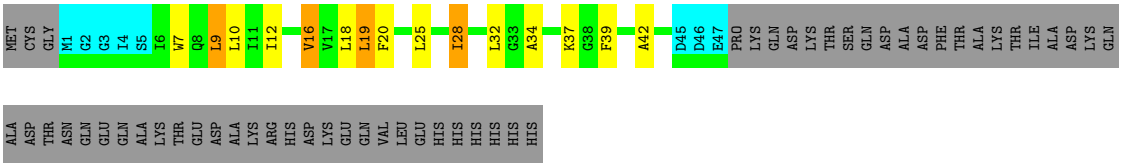
Chain A: 23% 16% • 7% 53%



4.2.9 Score per residue for model 9 (medoid)

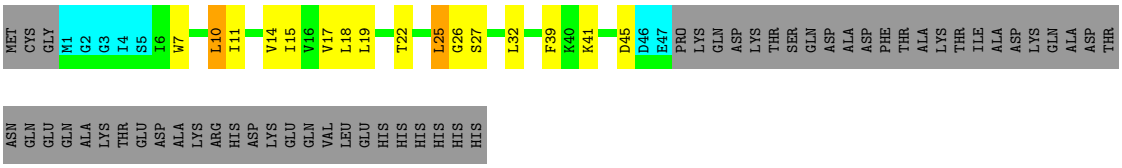
• Molecule 1: Sec-independent protein translocase protein TatA

Chain B: 24% 11% • 8% 53%



• Molecule 1: Sec-independent protein translocase protein TatA

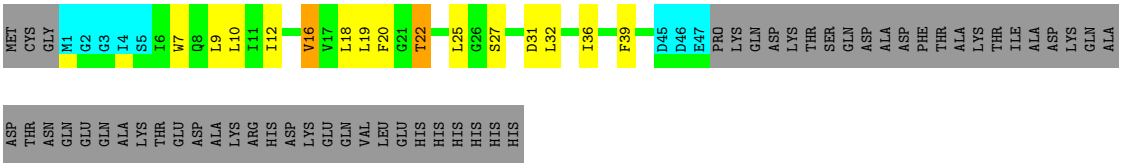
Chain A: 24% 14% • 7% 53%



4.2.10 Score per residue for model 10

• Molecule 1: Sec-independent protein translocase protein TatA

Chain B: 24% 13% • 8% 53%



• Molecule 1: Sec-independent protein translocase protein TatA

Chain A: 31% 9% 7% 53%

MET CYS GLY M1 G2 G3 I4 S5 I6 W7 L10 V14 V17 L18 T22 S27 K37 K41 D46 E47 PRO LYS GLN ASP LYS THR SER GLN ASP ALA ASP PHE THR ALA LYS THR ILE ALA ASP LYS GLN ALA ASP THR ASN GLN GLU GLN ALA LYS THR GLU

ASP ALA LYS ARG HIS ASP LYS GLU GLN VAL LEU GLU HIS HIS HIS HIS HIS HIS

5 Refinement protocol and experimental data overview (i)

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

Of the 100 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
X-PLOR NIH	refinement	
X-PLOR NIH	structure solution	

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	1096
Number of shifts mapped to atoms	606
Number of unparsed shifts	0
Number of shifts with mapping errors	490
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	49%

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	297	334	334	10±2
1	B	289	330	330	12±3
All	All	5860	6640	6640	148

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:20:PHE:CZ	1:A:17:VAL:HB	0.89	2.01	10	10
1:B:12:ILE:HG22	1:A:14:VAL:HG21	0.74	1.60	4	10
1:B:28:ILE:HG22	1:A:26:GLY:HA2	0.70	1.62	4	4
1:A:33:GLY:O	1:A:36:ILE:HG22	0.64	1.93	5	6
1:B:16:VAL:HG13	1:B:20:PHE:CE2	0.63	2.29	8	10
1:B:16:VAL:HG23	1:A:14:VAL:HG13	0.61	1.70	5	7
1:B:20:PHE:CE1	1:A:17:VAL:HB	0.59	2.33	2	8
1:B:39:PHE:CD1	1:A:40:LYS:HG2	0.58	2.33	5	3
1:B:36:ILE:HA	1:B:39:PHE:CE2	0.57	2.34	5	1
1:B:12:ILE:CG2	1:A:14:VAL:HG21	0.57	2.30	7	8
1:B:19:LEU:HD22	1:B:20:PHE:CE1	0.57	2.34	3	10
1:B:34:ALA:O	1:B:37:LYS:HG2	0.56	1.99	9	5
1:B:16:VAL:HG13	1:B:20:PHE:HE2	0.56	1.60	8	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:24:LYS:O	1:B:28:ILE:HG23	0.56	2.00	4	3
1:B:40:LYS:HA	1:B:43:MET:SD	0.56	2.41	6	1
1:B:28:ILE:HG22	1:A:26:GLY:CA	0.55	2.31	4	1
1:A:36:ILE:HA	1:A:39:PHE:CE2	0.54	2.37	5	1
1:A:17:VAL:HG13	1:A:25:LEU:HD13	0.53	1.79	3	3
1:A:37:LYS:O	1:A:41:LYS:HB2	0.52	2.04	7	6
1:A:17:VAL:HG13	1:A:25:LEU:HD11	0.52	1.80	9	1
1:A:24:LYS:O	1:A:28:ILE:HG22	0.51	2.05	1	2
1:B:33:GLY:O	1:B:36:ILE:HG22	0.50	2.06	6	5
1:B:42:ALA:O	1:A:44:SER:HB3	0.49	2.07	8	1
1:B:22:THR:HA	1:B:25:LEU:HD13	0.48	1.84	6	2
1:A:15:ILE:O	1:A:19:LEU:HG	0.48	2.09	2	6
1:B:39:PHE:CE1	1:A:40:LYS:HG2	0.47	2.44	3	1
1:B:9:LEU:HD13	1:A:10:LEU:CD1	0.46	2.40	9	3
1:B:9:LEU:HD13	1:A:10:LEU:HD12	0.46	1.88	9	3
1:A:17:VAL:HA	1:A:25:LEU:HD11	0.46	1.87	6	1
1:A:11:ILE:O	1:A:15:ILE:HG13	0.44	2.11	9	1
1:B:16:VAL:HG21	1:A:14:VAL:HG22	0.44	1.88	3	2
1:B:16:VAL:CG2	1:A:14:VAL:HG22	0.44	2.43	2	2
1:B:24:LYS:O	1:B:28:ILE:HG22	0.43	2.13	3	1
1:B:8:GLN:HG2	1:A:7:TRP:CH2	0.43	2.49	7	1
1:B:20:PHE:CE2	1:A:17:VAL:HB	0.43	2.47	2	1
1:A:34:ALA:O	1:A:37:LYS:HG2	0.42	2.14	6	1
1:B:42:ALA:CB	1:A:41:LYS:HA	0.42	2.45	9	1
1:B:20:PHE:HB3	1:A:22:THR:CG2	0.42	2.44	2	1
1:B:16:VAL:HG22	1:B:20:PHE:CE2	0.41	2.50	3	1
1:A:17:VAL:HG12	1:A:22:THR:HG22	0.41	1.90	4	1
1:A:17:VAL:HG13	1:A:25:LEU:CD1	0.41	2.46	1	1
1:B:37:LYS:O	1:B:41:LYS:HB2	0.41	2.16	8	1
1:B:41:LYS:HA	1:B:44:SER:OG	0.40	2.16	3	1
1:A:22:THR:HA	1:A:25:LEU:CD1	0.40	2.46	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	40/100 (40%)	37±1 (93±2%)	3±1 (7±2%)	0±0 (0±0%)	100	100
1	B	39/100 (39%)	37±1 (94±3%)	2±1 (5±3%)	0±0 (0±1%)	44	80
All	All	790/2000 (40%)	739 (94%)	50 (6%)	1 (0%)	54	85

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	B	23	LYS	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	32/83 (39%)	26±1 (81±5%)	6±1 (19±5%)	4	35
1	B	31/83 (37%)	22±1 (70±5%)	9±1 (30±5%)	1	16
All	All	630/1660 (38%)	475 (75%)	155 (25%)	2	25

All 32 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	B	9	LEU	10
1	B	18	LEU	10
1	A	10	LEU	10
1	A	18	LEU	10
1	B	32	LEU	9
1	B	39	PHE	9
1	B	7	TRP	8
1	A	7	TRP	8
1	B	16	VAL	7
1	B	19	LEU	6
1	A	39	PHE	5
1	B	22	THR	5
1	A	16	VAL	4
1	A	32	LEU	4
1	B	10	LEU	4
1	A	9	LEU	4

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Mol	Chain	Res	Type	Models (Total)
1	B	31	ASP	4
1	B	25	LEU	4
1	B	27	SER	4
1	A	27	SER	4
1	A	44	SER	3
1	B	24	LYS	3
1	A	22	THR	3
1	A	31	ASP	3
1	B	28	ILE	3
1	B	43	MET	2
1	B	44	SER	2
1	B	36	ILE	2
1	A	25	LEU	2
1	B	30	SER	1
1	A	11	ILE	1
1	A	45	ASP	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 monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 49% for the well-defined parts and 48% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1096
Number of shifts mapped to atoms	606
Number of unparsed shifts	0
Number of shifts with mapping errors	490
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. All 490 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	48	PRO	CA	63.224	.	1
1	A	48	PRO	HA	4.389	.	1
1	A	48	PRO	CB	32.073	.	1
1	A	48	PRO	HB2	2.26	.	2
1	A	48	PRO	HB3	1.852	.	2
1	A	48	PRO	CG	27.45	.	1
1	A	48	PRO	HG2	2.015	.	2
1	A	48	PRO	HG3	1.98	.	2
1	A	48	PRO	CD	50.712	.	1
1	A	48	PRO	HD2	3.79	.	2
1	A	48	PRO	HD3	3.645	.	2
1	A	48	PRO	C	176.94	.	1
1	A	49	LYS	N	122.672	.	1
1	A	49	LYS	H	8.373	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	49	LYS	CA	56.362	.	1
1	A	49	LYS	HA	4.255	.	1
1	A	49	LYS	CB	32.86	.	1
1	A	49	LYS	HB2	1.755	.	2
1	A	49	LYS	HB3	1.671	.	2
1	A	49	LYS	CG	24.68	.	1
1	A	49	LYS	HG2	1.389	.	2
1	A	49	LYS	HG3	1.389	.	2
1	A	49	LYS	CD	29.08	.	1
1	A	49	LYS	HD2	1.602	.	2
1	A	49	LYS	HD3	1.602	.	2
1	A	49	LYS	CE	42.25	.	1
1	A	49	LYS	HE2	2.925	.	2
1	A	49	LYS	HE3	2.925	.	2
1	A	49	LYS	C	176.83	.	1
1	A	50	GLN	N	122.296	.	1
1	A	50	GLN	H	8.363	.	1
1	A	50	GLN	CA	55.81	.	1
1	A	50	GLN	HA	4.294	.	1
1	A	50	GLN	CB	29.59	.	1
1	A	50	GLN	HB2	1.992	.	2
1	A	50	GLN	HB3	1.87	.	2
1	A	50	GLN	CG	33.86	.	1
1	A	50	GLN	HG2	2.276	.	2
1	A	50	GLN	HG3	2.276	.	2
1	A	50	GLN	NE2	113.35	.	1
1	A	50	GLN	HE21	7.487	.	2
1	A	50	GLN	HE22	6.784	.	2
1	A	50	GLN	C	175.59	.	1
1	A	51	ASP	N	122.524	.	1
1	A	51	ASP	H	8.375	.	1
1	A	51	ASP	CA	54.33	.	1
1	A	51	ASP	HA	4.519	.	1
1	A	51	ASP	CB	41.28	.	1
1	A	51	ASP	HB2	2.63	.	2
1	A	51	ASP	HB3	2.527	.	2
1	A	51	ASP	C	176.36	.	1
1	A	52	LYS	N	122.679	.	1
1	A	52	LYS	H	8.305	.	1
1	A	52	LYS	CA	56.39	.	1
1	A	52	LYS	HA	4.323	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	52	LYS	CB	32.84	.	1
1	A	52	LYS	HB2	1.806	.	2
1	A	52	LYS	HB3	1.688	.	2
1	A	52	LYS	CG	24.73	.	1
1	A	52	LYS	HG2	1.37	.	2
1	A	52	LYS	HG3	1.37	.	2
1	A	52	LYS	CD	28.81	.	1
1	A	52	LYS	HD2	1.597	.	2
1	A	52	LYS	HD3	1.597	.	2
1	A	52	LYS	CE	42.15	.	1
1	A	52	LYS	HE2	2.918	.	2
1	A	52	LYS	HE3	2.918	.	2
1	A	52	LYS	C	177.06	.	1
1	A	53	THR	N	115.365	.	1
1	A	53	THR	H	8.23	.	1
1	A	53	THR	CA	62.48	.	1
1	A	53	THR	HA	4.26	.	1
1	A	53	THR	CB	69.83	.	1
1	A	53	THR	HB	4.184	.	1
1	A	53	THR	CG2	21.55	.	1
1	A	53	THR	HG21	1.136	.	1
1	A	53	THR	HG22	1.136	.	1
1	A	53	THR	HG23	1.136	.	1
1	A	53	THR	C	175.04	.	1
1	A	54	SER	N	118.458	.	1
1	A	54	SER	H	8.212	.	1
1	A	54	SER	CA	58.66	.	1
1	A	54	SER	HA	4.409	.	1
1	A	54	SER	CB	63.77	.	1
1	A	54	SER	HB2	3.849	.	2
1	A	54	SER	HB3	3.777	.	2
1	A	54	SER	C	174.71	.	1
1	A	55	GLN	N	122.66	.	1
1	A	55	GLN	H	8.296	.	1
1	A	55	GLN	CA	56.23	.	1
1	A	55	GLN	HA	4.247	.	1
1	A	55	GLN	CB	29.42	.	1
1	A	55	GLN	HB2	2.04	.	2
1	A	55	GLN	HB3	1.887	.	2
1	A	55	GLN	CG	33.87	.	1
1	A	55	GLN	HG2	2.255	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	55	GLN	HG3	2.255	.	2
1	A	55	GLN	C	175.91	.	1
1	A	56	ASP	N	121.97	.	1
1	A	56	ASP	H	8.219	.	1
1	A	56	ASP	CA	54.63	.	1
1	A	56	ASP	HA	4.524	.	1
1	A	56	ASP	CB	40.96	.	1
1	A	56	ASP	HB2	2.534	.	2
1	A	56	ASP	HB3	2.534	.	2
1	A	56	ASP	C	176.32	.	1
1	A	57	ALA	N	124.711	.	1
1	A	57	ALA	H	8.104	.	1
1	A	57	ALA	CA	53.01	.	1
1	A	57	ALA	HA	4.203	.	1
1	A	57	ALA	CB	19.09	.	1
1	A	57	ALA	HB1	1.263	.	1
1	A	57	ALA	HB2	1.263	.	1
1	A	57	ALA	HB3	1.263	.	1
1	A	57	ALA	C	177.58	.	1
1	A	58	ASP	N	119.512	.	1
1	A	58	ASP	H	8.127	.	1
1	A	58	ASP	CA	54.29	.	1
1	A	58	ASP	HA	4.533	.	1
1	A	58	ASP	CB	41.04	.	1
1	A	58	ASP	HB2	2.573	.	2
1	A	58	ASP	HB3	2.491	.	2
1	A	58	ASP	C	176.55	.	1
1	A	59	PHE	N	121.824	.	1
1	A	59	PHE	H	8.084	.	1
1	A	59	PHE	CA	58.43	.	1
1	A	59	PHE	HA	4.55	.	1
1	A	59	PHE	CB	39.31	.	1
1	A	59	PHE	HB2	3.169	.	2
1	A	59	PHE	HB3	3.08	.	2
1	A	59	PHE	HD1	7.23	.	2
1	A	59	PHE	C	176.47	.	1
1	A	60	THR	N	116.191	.	1
1	A	60	THR	H	8.015	.	1
1	A	60	THR	CA	62.78	.	1
1	A	60	THR	HA	4.146	.	1
1	A	60	THR	CB	69.776	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	60	THR	HB	4.151	.	1
1	A	60	THR	CG2	21.59	.	1
1	A	60	THR	HG21	1.157	.	1
1	A	60	THR	HG22	1.157	.	1
1	A	60	THR	HG23	1.157	.	1
1	A	60	THR	C	174.46	.	1
1	A	61	ALA	N	126.467	.	1
1	A	61	ALA	H	8.046	.	1
1	A	61	ALA	CA	53.01	.	1
1	A	61	ALA	HA	4.139	.	1
1	A	61	ALA	CB	18.97	.	1
1	A	61	ALA	HB1	1.371	.	1
1	A	61	ALA	HB2	1.371	.	1
1	A	61	ALA	HB3	1.371	.	1
1	A	61	ALA	C	178.03	.	1
1	A	62	LYS	N	120.805	.	1
1	A	62	LYS	H	8.081	.	1
1	A	62	LYS	CA	56.62	.	1
1	A	62	LYS	HA	4.257	.	1
1	A	62	LYS	CB	33.01	.	1
1	A	62	LYS	HB2	1.767	.	2
1	A	62	LYS	HB3	1.7	.	2
1	A	62	LYS	CG	24.77	.	1
1	A	62	LYS	HG2	1.392	.	2
1	A	62	LYS	HG3	1.392	.	2
1	A	62	LYS	CD	29.04	.	1
1	A	62	LYS	HD2	1.597	.	2
1	A	62	LYS	HD3	1.597	.	2
1	A	62	LYS	CE	42.2	.	1
1	A	62	LYS	HE2	2.922	.	2
1	A	62	LYS	HE3	2.922	.	2
1	A	62	LYS	C	177.16	.	1
1	A	63	THR	N	115.956	.	1
1	A	63	THR	H	8.055	.	1
1	A	63	THR	CA	62.224	.	1
1	A	63	THR	HA	4.273	.	1
1	A	63	THR	CB	69.78	.	1
1	A	63	THR	HB	4.146	.	1
1	A	63	THR	CG2	21.55	.	1
1	A	63	THR	HG21	1.152	.	1
1	A	63	THR	HG22	1.152	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	63	THR	HG23	1.152	.	1
1	A	63	THR	C	174.88	.	1
1	A	64	ILE	N	123.467	.	1
1	A	64	ILE	H	8.036	.	1
1	A	64	ILE	CA	61.57	.	1
1	A	64	ILE	HA	4.092	.	1
1	A	64	ILE	CB	38.57	.	1
1	A	64	ILE	HB	1.838	.	1
1	A	64	ILE	CG1	27.46	.	2
1	A	64	ILE	HG12	1.444	.	9
1	A	64	ILE	HG13	1.158	.	9
1	A	64	ILE	CD1	12.94	.	1
1	A	64	ILE	HD11	0.87	.	1
1	A	64	ILE	HD12	0.87	.	1
1	A	64	ILE	HD13	0.87	.	1
1	A	64	ILE	CG2	17.42	.	2
1	A	64	ILE	HG21	0.833	.	4
1	A	64	ILE	HG22	0.833	.	4
1	A	64	ILE	HG23	0.833	.	4
1	A	64	ILE	C	176.24	.	1
1	A	65	ALA	N	127.935	.	1
1	A	65	ALA	H	8.169	.	1
1	A	65	ALA	CA	52.84	.	1
1	A	65	ALA	HA	4.201	.	1
1	A	65	ALA	CB	19.27	.	1
1	A	65	ALA	HB1	1.356	.	1
1	A	65	ALA	HB2	1.356	.	1
1	A	65	ALA	HB3	1.356	.	1
1	A	65	ALA	C	177.83	.	1
1	A	66	ASP	N	120.412	.	1
1	A	66	ASP	H	8.145	.	1
1	A	66	ASP	CA	54.61	.	1
1	A	66	ASP	HA	4.463	.	1
1	A	66	ASP	CB	41.18	.	1
1	A	66	ASP	HB2	2.58	.	2
1	A	66	ASP	HB3	2.58	.	2
1	A	66	ASP	C	176.47	.	1
1	A	67	LYS	N	121.507	.	1
1	A	67	LYS	H	8.16	.	1
1	A	67	LYS	CA	56.58	.	1
1	A	67	LYS	HA	4.161	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	67	LYS	CB	32.89	.	1
1	A	67	LYS	HB2	1.773	.	2
1	A	67	LYS	HB3	1.696	.	2
1	A	67	LYS	CG	24.98	.	1
1	A	67	LYS	HG2	1.407	.	2
1	A	67	LYS	HG3	1.407	.	2
1	A	67	LYS	CD	29.1	.	1
1	A	67	LYS	HD2	1.602	.	2
1	A	67	LYS	HD3	1.602	.	2
1	A	67	LYS	CE	41.95	.	1
1	A	67	LYS	HE2	2.924	.	2
1	A	67	LYS	HE3	2.924	.	2
1	A	67	LYS	C	176.93	.	1
1	A	68	GLN	N	121.715	.	1
1	A	68	GLN	H	8.274	.	1
1	A	68	GLN	CA	56.15	.	1
1	A	68	GLN	HA	4.188	.	1
1	A	68	GLN	CB	29.38	.	1
1	A	68	GLN	HB2	2.028	.	2
1	A	68	GLN	HB3	1.925	.	2
1	A	68	GLN	CG	33.86	.	1
1	A	68	GLN	HG2	2.307	.	2
1	A	68	GLN	HG3	2.307	.	2
1	A	68	GLN	C	176.01	.	1
1	A	69	ALA	N	125.438	.	1
1	A	69	ALA	H	8.172	.	1
1	A	69	ALA	CA	52.78	.	1
1	A	69	ALA	HA	4.261	.	1
1	A	69	ALA	CB	19.29	.	1
1	A	69	ALA	HB1	1.321	.	1
1	A	69	ALA	HB2	1.321	.	1
1	A	69	ALA	HB3	1.321	.	1
1	A	69	ALA	C	177.65	.	1
1	A	70	ASP	N	120.383	.	1
1	A	70	ASP	H	8.237	.	1
1	A	70	ASP	CA	54.53	.	1
1	A	70	ASP	HA	4.532	.	1
1	A	70	ASP	CB	41.16	.	1
1	A	70	ASP	HB2	2.665	.	2
1	A	70	ASP	HB3	2.569	.	2
1	A	70	ASP	C	176.85	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	71	THR	N	114.569	.	1
1	A	71	THR	H	8.026	.	1
1	A	71	THR	CA	62.22	.	1
1	A	71	THR	HA	4.295	.	1
1	A	71	THR	CB	69.56	.	1
1	A	71	THR	HB	4.295	.	1
1	A	71	THR	CG2	21.59	.	1
1	A	71	THR	HG21	1.183	.	1
1	A	71	THR	HG22	1.183	.	1
1	A	71	THR	HG23	1.183	.	1
1	A	71	THR	C	174.81	.	1
1	A	72	ASN	N	121.47	.	1
1	A	72	ASN	H	8.408	.	1
1	A	72	ASN	CA	53.75	.	1
1	A	72	ASN	HA	4.622	.	1
1	A	72	ASN	CB	38.82	.	1
1	A	72	ASN	HB2	2.786	.	2
1	A	72	ASN	HB3	2.741	.	2
1	A	72	ASN	C	175.58	.	1
1	A	73	GLN	N	121.367	.	1
1	A	73	GLN	H	8.276	.	1
1	A	73	GLN	CA	56.42	.	1
1	A	73	GLN	HA	4.273	.	1
1	A	73	GLN	CB	29.39	.	1
1	A	73	GLN	HB2	2.056	.	2
1	A	73	GLN	HB3	1.911	.	2
1	A	73	GLN	CG	33.83	.	1
1	A	73	GLN	HG2	2.289	.	2
1	A	73	GLN	HG3	2.289	.	2
1	A	73	GLN	C	176.44	.	1
1	A	74	GLU	N	122.508	.	1
1	A	74	GLU	H	8.34	.	1
1	A	74	GLU	CA	56.99	.	1
1	A	74	GLU	HA	4.136	.	1
1	A	74	GLU	CB	29.84	.	1
1	A	74	GLU	HB2	1.979	.	2
1	A	74	GLU	HB3	1.906	.	2
1	A	74	GLU	CG	36.25	.	1
1	A	74	GLU	HG2	2.203	.	2
1	A	74	GLU	HG3	2.203	.	2
1	A	75	GLN	H	8.289	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	75	GLN	CA	56.15	.	1
1	A	75	GLN	HA	4.186	.	1
1	A	75	GLN	CB	29.22	.	1
1	A	75	GLN	HB2	2.034	.	2
1	A	75	GLN	HB3	1.911	.	2
1	A	75	GLN	CG	33.822	.	1
1	A	75	GLN	HG2	2.312	.	2
1	A	75	GLN	HG3	2.312	.	2
1	A	76	ALA	N	125.639	.	1
1	A	76	ALA	H	8.192	.	1
1	A	76	ALA	CA	52.89	.	1
1	A	76	ALA	HA	4.201	.	1
1	A	76	ALA	CB	19.08	.	1
1	A	76	ALA	HB1	1.358	.	1
1	A	76	ALA	HB2	1.358	.	1
1	A	76	ALA	HB3	1.358	.	1
1	A	76	ALA	C	178.07	.	1
1	A	77	LYS	N	121.348	.	1
1	A	77	LYS	H	8.222	.	1
1	A	77	LYS	CA	56.55	.	1
1	A	77	LYS	HA	4.252	.	1
1	A	77	LYS	CB	32.95	.	1
1	A	77	LYS	HB2	1.771	.	2
1	A	77	LYS	HB3	1.702	.	2
1	A	77	LYS	CG	24.73	.	1
1	A	77	LYS	HG2	1.359	.	2
1	A	77	LYS	HG3	1.359	.	2
1	A	77	LYS	CD	29.1	.	1
1	A	77	LYS	HD2	1.607	.	2
1	A	77	LYS	HD3	1.607	.	2
1	A	77	LYS	CE	42.215	.	1
1	A	77	LYS	HE2	2.922	.	2
1	A	77	LYS	HE3	2.922	.	2
1	A	78	THR	N	115.941	.	1
1	A	78	THR	H	8.07	.	1
1	A	78	THR	CA	62.27	.	1
1	A	78	THR	HA	4.23	.	1
1	A	78	THR	CB	69.77	.	1
1	A	78	THR	HB	4.202	.	1
1	A	78	THR	CG2	21.59	.	1
1	A	78	THR	HG21	1.14	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	78	THR	HG22	1.14	.	1
1	A	78	THR	HG23	1.14	.	1
1	A	78	THR	C	175.05	.	1
1	A	79	GLU	N	123.459	.	1
1	A	79	GLU	H	8.444	.	1
1	A	79	GLU	CA	57.24	.	1
1	A	79	GLU	HA	4.191	.	1
1	A	79	GLU	CB	30.1	.	1
1	A	79	GLU	HB2	1.973	.	2
1	A	79	GLU	HB3	1.901	.	2
1	A	79	GLU	CG	36.18	.	1
1	A	79	GLU	HG2	2.212	.	2
1	A	79	GLU	HG3	2.212	.	2
1	A	79	GLU	C	176.93	.	1
1	A	80	ASP	N	121.69	.	1
1	A	80	ASP	H	8.273	.	1
1	A	80	ASP	CA	55.09	.	1
1	A	80	ASP	HA	4.514	.	1
1	A	80	ASP	CB	41.2	.	1
1	A	80	ASP	HB2	2.579	.	2
1	A	80	ASP	HB3	2.579	.	2
1	A	80	ASP	C	176.69	.	1
1	A	81	ALA	N	124.69	.	1
1	A	81	ALA	H	8.084	.	1
1	A	81	ALA	CA	52.984	.	1
1	A	81	ALA	HA	4.216	.	1
1	A	81	ALA	CB	19.04	.	1
1	A	81	ALA	HB1	1.358	.	1
1	A	81	ALA	HB2	1.358	.	1
1	A	81	ALA	HB3	1.358	.	1
1	A	81	ALA	C	178.35	.	1
1	A	82	LYS	N	119.788	.	1
1	A	82	LYS	H	8.042	.	1
1	A	82	LYS	CA	56.65	.	1
1	A	82	LYS	HA	4.205	.	1
1	A	82	LYS	CB	32.72	.	1
1	A	82	LYS	HB2	1.746	.	2
1	A	82	LYS	HB3	1.746	.	2
1	A	82	LYS	CG	24.76	.	1
1	A	82	LYS	HG2	1.352	.	2
1	A	82	LYS	HG3	1.352	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	82	LYS	CD	29.06	.	1
1	A	82	LYS	HD2	1.603	.	2
1	A	82	LYS	HD3	1.603	.	2
1	A	82	LYS	CE	42.16	.	1
1	A	82	LYS	HE2	2.918	.	2
1	A	82	LYS	HE3	2.918	.	2
1	A	82	LYS	C	176.91	.	1
1	A	83	ARG	N	121.675	.	1
1	A	83	ARG	H	7.964	.	1
1	A	83	ARG	CA	56.56	.	1
1	A	83	ARG	HA	4.139	.	1
1	A	83	ARG	CB	30.61	.	1
1	A	83	ARG	HB2	1.733	.	2
1	A	83	ARG	HB3	1.693	.	2
1	A	83	ARG	CG	27.18	.	1
1	A	83	ARG	HG2	1.536	.	2
1	A	83	ARG	HG3	1.47	.	2
1	A	83	ARG	CD	43.32	.	1
1	A	83	ARG	HD2	3.149	.	2
1	A	83	ARG	HD3	3.149	.	2
1	A	84	HIS	H	8.211	.	1
1	A	84	HIS	CA	56.04	.	1
1	A	84	HIS	HA	4.599	.	1
1	A	84	HIS	CB	29.36	.	1
1	A	84	HIS	HB2	3.201	.	2
1	A	84	HIS	HB3	3.065	.	2
1	A	85	ASP	N	122.377	.	1
1	A	85	ASP	H	8.237	.	1
1	A	85	ASP	CA	54.7	.	1
1	A	85	ASP	HA	4.531	.	1
1	A	85	ASP	CB	41.23	.	1
1	A	85	ASP	HB2	2.577	.	2
1	A	85	ASP	HB3	2.548	.	2
1	A	86	LYS	N	121.916	.	1
1	A	86	LYS	H	8.085	.	1
1	A	86	LYS	CA	56.54	.	1
1	A	86	LYS	HA	4.256	.	1
1	A	86	LYS	CB	32.72	.	1
1	A	86	LYS	HB2	1.843	.	2
1	A	86	LYS	HB3	1.843	.	2
1	A	86	LYS	CG	24.7	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	86	LYS	HG2	1.362	.	2
1	A	86	LYS	HG3	1.362	.	2
1	A	86	LYS	CD	29.25	.	1
1	A	86	LYS	HD2	1.61	.	2
1	A	86	LYS	HD3	1.61	.	2
1	A	86	LYS	CE	42.2	.	1
1	A	86	LYS	HE2	2.921	.	2
1	A	86	LYS	HE3	2.921	.	2
1	A	87	GLU	CA	56.77	.	1
1	A	87	GLU	HA	4.233	.	1
1	A	87	GLU	CB	30.05	.	1
1	A	87	GLU	HB2	1.967	.	2
1	A	87	GLU	HB3	1.905	.	2
1	A	87	GLU	CG	36.31	.	1
1	A	87	GLU	HG2	2.212	.	2
1	A	87	GLU	HG3	2.212	.	2
1	A	88	GLN	N	121.927	.	1
1	A	88	GLN	H	8.273	.	1
1	A	88	GLN	CA	55.83	.	1
1	A	88	GLN	HA	4.297	.	1
1	A	88	GLN	CB	29.7	.	1
1	A	88	GLN	HB2	1.977	.	2
1	A	88	GLN	HB3	1.882	.	2
1	A	88	GLN	CG	33.86	.	1
1	A	88	GLN	HG2	2.272	.	2
1	A	88	GLN	HG3	2.272	.	2
1	A	88	GLN	C	175.96	.	1
1	A	89	VAL	N	122.589	.	1
1	A	89	VAL	H	8.099	.	1
1	A	89	VAL	CA	62.56	.	1
1	A	89	VAL	HA	4.033	.	1
1	A	89	VAL	CB	32.719	.	1
1	A	89	VAL	HB	2.012	.	1
1	A	89	VAL	CG2	21.072	.	2
1	A	89	VAL	HG21	0.905	.	4
1	A	89	VAL	HG22	0.905	.	4
1	A	89	VAL	HG23	0.905	.	4
1	A	89	VAL	C	176.18	.	1
1	A	90	LEU	N	126.509	.	1
1	A	90	LEU	H	8.21	.	1
1	A	90	LEU	CA	55.11	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	90	LEU	HA	4.304	.	1
1	A	90	LEU	CB	42.27	.	1
1	A	90	LEU	HB2	1.542	.	2
1	A	90	LEU	HB3	1.454	.	2
1	A	90	LEU	CG	26.96	.	1
1	A	90	LEU	HG	1.492	.	1
1	A	90	LEU	HD11	0.851	.	4
1	A	90	LEU	HD12	0.851	.	4
1	A	90	LEU	HD13	0.851	.	4
1	A	90	LEU	CD2	23.706	.	2
1	A	90	LEU	HD21	0.795	.	4
1	A	90	LEU	HD22	0.795	.	4
1	A	90	LEU	HD23	0.795	.	4
1	A	90	LEU	C	175.91	.	1
1	A	91	GLU	N	122.152	.	1
1	A	91	GLU	H	8.203	.	1
1	A	91	GLU	CA	56.46	.	1
1	A	91	GLU	HA	4.2	.	1
1	A	91	GLU	CB	30.3	.	1
1	A	91	GLU	HB2	1.996	.	2
1	A	91	GLU	HB3	1.85	.	2
1	A	91	GLU	CG	36.14	.	1
1	A	91	GLU	HG2	2.203	.	2
1	A	91	GLU	HG3	2.203	.	2
1	A	91	GLU	C	175.7	.	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	91	-0.40 ± 0.38	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	84	0.07 ± 0.16	None needed (< 0.5 ppm)
$^{13}C'$	80	-0.18 ± 0.29	None needed (< 0.5 ppm)
^{15}N	87	0.40 ± 0.29	None needed (< 0.5 ppm)

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 49%, i.e. 536 atoms were assigned a chemical shift out of a possible 1101. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	203/405 (50%)	84/168 (50%)	79/158 (50%)	40/79 (51%)
Sidechain	310/632 (49%)	213/424 (50%)	96/196 (49%)	1/12 (8%)
Aromatic	23/64 (36%)	12/32 (38%)	10/30 (33%)	1/2 (50%)
Overall	536/1101 (49%)	309/624 (50%)	185/384 (48%)	42/93 (45%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 48%, i.e. 606 atoms were assigned a chemical shift out of a possible 1258. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	238/484 (49%)	100/202 (50%)	91/188 (48%)	47/94 (50%)
Sidechain	345/710 (49%)	237/474 (50%)	107/224 (48%)	1/12 (8%)
Aromatic	23/64 (36%)	12/32 (38%)	10/30 (33%)	1/2 (50%)
Overall	606/1258 (48%)	349/708 (49%)	208/442 (47%)	49/108 (45%)

7.1.4 Statistically unusual chemical shifts (i)

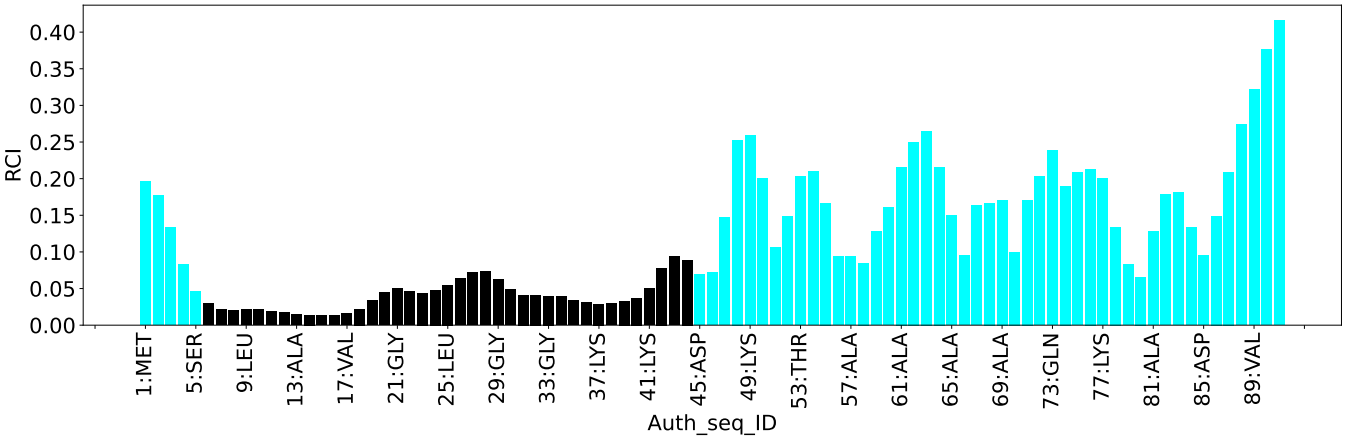
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	7	TRP	CB	41.32	20.06 – 39.75	5.8

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:


RCI
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
1:MET
5:SER
9:LEU
13:ALA
17:VAL
21:GLY
25:LEU
29:GLY
33:GLY
37:LYS
41:LYS
45:ASP
49:LYS
53:THR
57:ALA
61:ALA
65:ALA
69:ALA
73:GLN
77:LYS
81:ALA
85:ASP
89:VAL
Auth_seq_ID