



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2JUC / pdb_00002juc
BMRB ID : 15439
Title : URN1 FF domain yeast
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Deposited on : 2007-08-21

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

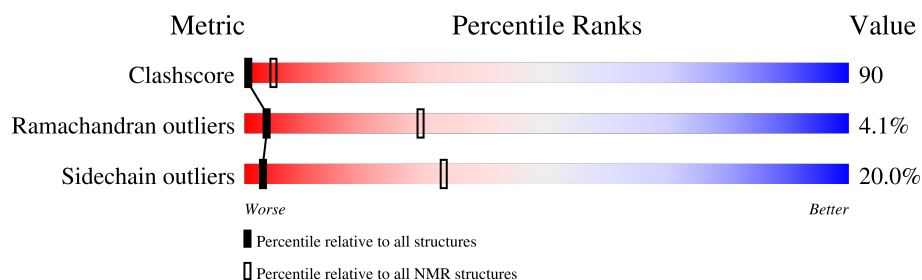
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 48%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	59	27% 39% 20% • • 7%

2 Ensemble composition and analysis

This entry contains 15 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:7-A:59 (53)	0.48	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 3 clusters. No single-model clusters were found.

Cluster number	Models
1	2, 4, 5, 6, 9, 13, 15
2	1, 3, 7, 10, 11
3	8, 12, 14

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 935 atoms, of which 449 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Pre-mRNA-splicing factor URN1.

Mol	Chain	Residues	Atoms							Trace
1	A	55	Total	C	H	N	O	S		0
			935	311	449	77	97	1		

There are 4 discrepancies between the modelled and reference sequences:

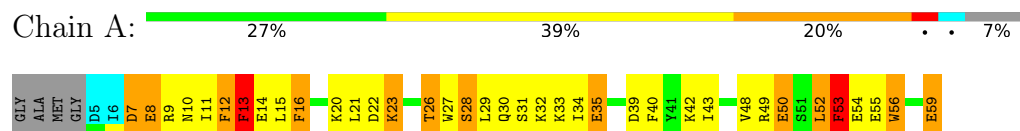
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q06525
A	2	ALA	-	expression tag	UNP Q06525
A	3	MET	-	expression tag	UNP Q06525
A	4	GLY	-	expression tag	UNP Q06525

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: Pre-mRNA-splicing factor URN1

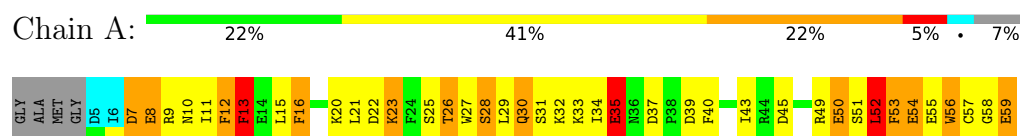


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

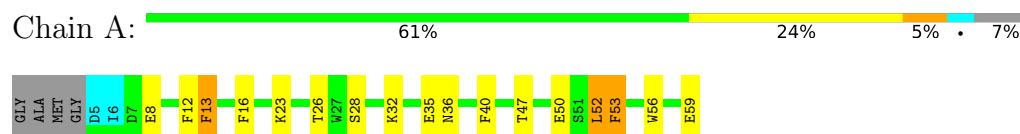
4.2.1 Score per residue for model 1

- Molecule 1: Pre-mRNA-splicing factor URN1



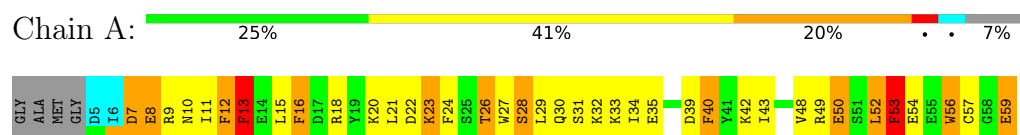
4.2.2 Score per residue for model 2

- Molecule 1: Pre-mRNA-splicing factor URN1



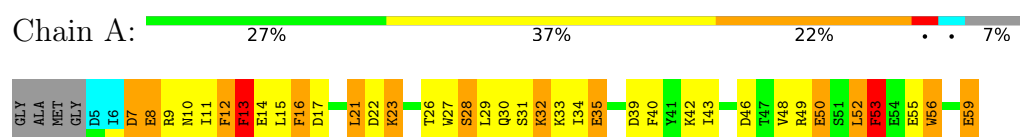
4.2.3 Score per residue for model 3

- Molecule 1: Pre-mRNA-splicing factor URN1



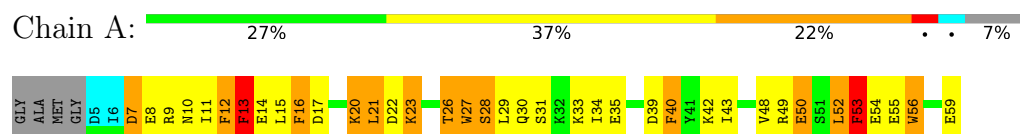
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Pre-mRNA-splicing factor URN1



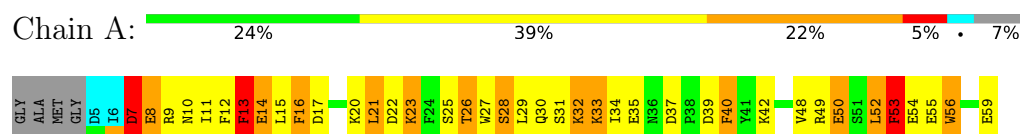
4.2.5 Score per residue for model 5

- Molecule 1: Pre-mRNA-splicing factor URN1



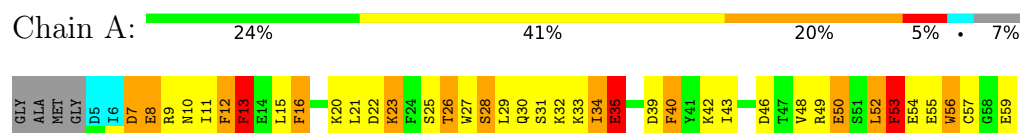
4.2.6 Score per residue for model 6

- Molecule 1: Pre-mRNA-splicing factor URN1



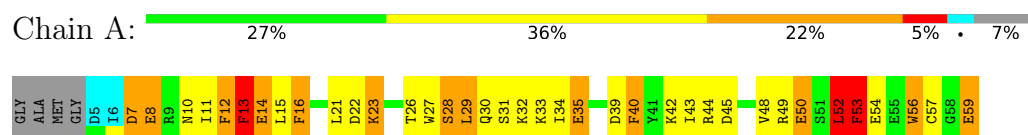
4.2.7 Score per residue for model 7

- Molecule 1: Pre-mRNA-splicing factor URN1



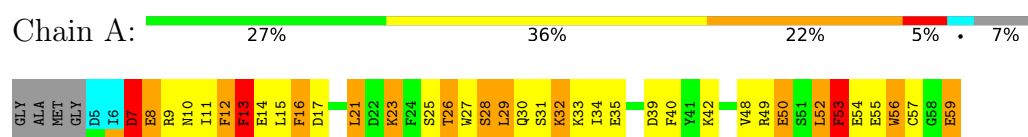
4.2.8 Score per residue for model 8

- Molecule 1: Pre-mRNA-splicing factor URN1



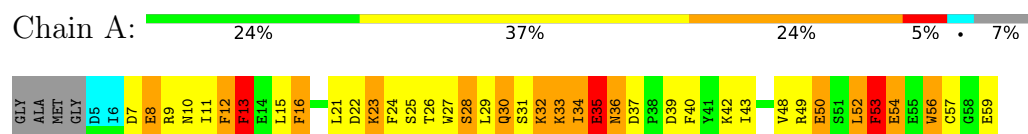
4.2.9 Score per residue for model 9

- Molecule 1: Pre-mRNA-splicing factor URN1



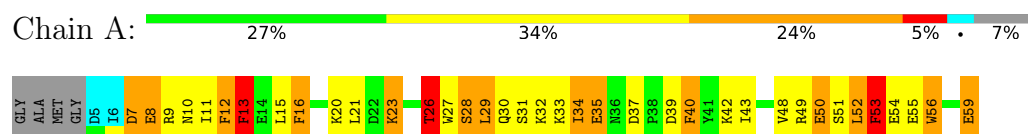
4.2.10 Score per residue for model 10

- Molecule 1: Pre-mRNA-splicing factor URN1



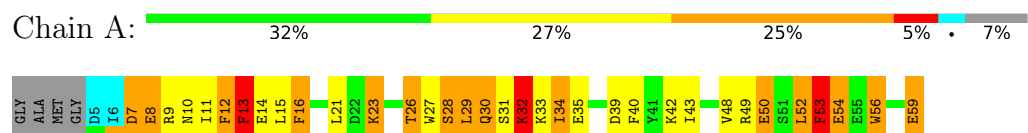
4.2.11 Score per residue for model 11

- Molecule 1: Pre-mRNA-splicing factor URN1



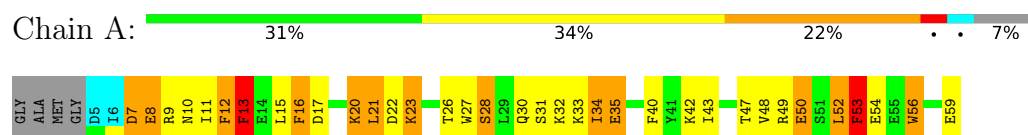
4.2.12 Score per residue for model 12

- Molecule 1: Pre-mRNA-splicing factor URN1



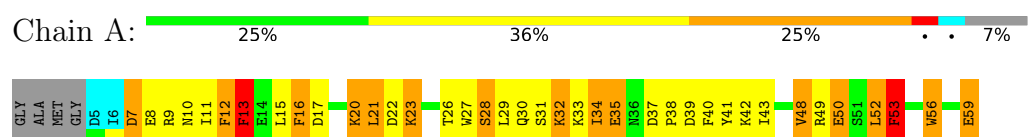
4.2.13 Score per residue for model 13

- Molecule 1: Pre-mRNA-splicing factor URN1



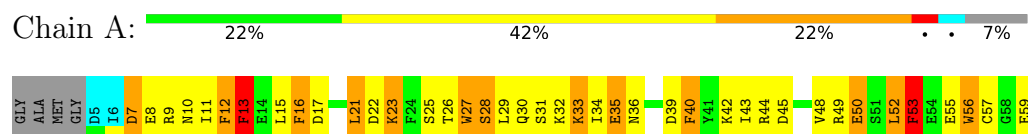
4.2.14 Score per residue for model 14

- Molecule 1: Pre-mRNA-splicing factor URN1



4.2.15 Score per residue for model 15

- Molecule 1: Pre-mRNA-splicing factor URN1



5 Refinement protocol and experimental data overview

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

Of the 60 calculated structures, 15 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	refinement	

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	397
Number of shifts mapped to atoms	385
Number of unparsed shifts	0
Number of shifts with mapping errors	12
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	48%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.52±0.02	11±1/482 (2.4± 0.2%)	1.46±0.02	7±1/645 (1.1± 0.2%)
All	All	1.52	172/7191 (2.4%)	1.46	103/9621 (1.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	56	TRP	CD2-CE3	-13.52	1.18	1.40	2	15
1	A	52	LEU	C-N	-10.67	1.20	1.33	2	15
1	A	7	ASP	C-N	-10.61	1.20	1.33	9	14
1	A	56	TRP	CG-CD2	-10.45	1.25	1.43	8	15
1	A	56	TRP	NE1-CE2	-8.30	1.28	1.37	10	15
1	A	53	PHE	N-CA	-8.29	1.36	1.46	2	15
1	A	13	PHE	CA-CB	-7.09	1.42	1.53	7	15
1	A	56	TRP	CE3-CZ3	-6.67	1.18	1.38	8	15
1	A	28	SER	CA-CB	-6.33	1.43	1.53	11	14
1	A	12	PHE	C-O	-5.96	1.17	1.24	15	14
1	A	53	PHE	CA-CB	-5.52	1.44	1.53	3	8
1	A	16	PHE	N-CA	-5.50	1.39	1.46	4	6
1	A	26	THR	CA-C	-5.37	1.46	1.52	3	4
1	A	27	TRP	NE1-CE2	-5.36	1.31	1.37	15	2
1	A	52	LEU	CA-C	-5.27	1.46	1.52	9	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	53	PHE	N-CA-CB	-13.23	90.22	110.06	1	15
1	A	56	TRP	CG-CD2-CE3	-10.06	123.84	133.90	8	15
1	A	13	PHE	CA-CB-CG	9.55	123.35	113.80	2	15
1	A	16	PHE	CA-CB-CG	9.51	123.31	113.80	5	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	28	SER	N-CA-C	6.61	120.56	112.23	11	8
1	A	52	LEU	CA-C-N	5.91	128.48	120.38	1	2
1	A	52	LEU	C-N-CA	5.91	128.48	120.38	1	2
1	A	56	TRP	CB-CG-CD1	5.77	135.56	126.90	8	5
1	A	13	PHE	CB-CA-C	-5.68	101.30	110.74	13	4
1	A	40	PHE	CA-CB-CG	5.66	119.46	113.80	11	1
1	A	56	TRP	CB-CG-CD2	-5.48	119.13	126.80	8	2
1	A	13	PHE	N-CA-CB	-5.47	101.25	110.49	10	1
1	A	32	LYS	N-CA-C	-5.35	106.71	113.18	12	2
1	A	52	LEU	CA-C-O	5.27	126.19	120.55	2	4
1	A	56	TRP	CE2-CD2-CG	5.22	113.47	107.20	2	2
1	A	56	TRP	CE3-CZ3-CH2	5.22	127.89	121.10	4	8
1	A	29	LEU	N-CA-C	-5.21	105.09	111.75	12	1
1	A	48	VAL	N-CA-C	-5.12	108.51	113.53	14	1

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	470	434	434	79±22
All	All	7050	6510	6076	1180

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 90.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:PHE:HB3	1:A:56:TRP:CD1	1.05	1.86	1	14
1:A:27:TRP:CD2	1:A:50:GLU:HB3	1.04	1.87	12	14
1:A:16:PHE:HB3	1:A:56:TRP:CZ3	0.99	1.91	1	14
1:A:31:SER:HA	1:A:34:ILE:HD11	0.99	1.30	13	4
1:A:16:PHE:HB3	1:A:56:TRP:CH2	0.98	1.93	9	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:TRP:HA	1:A:59:GLU:HB2	0.96	1.37	7	13
1:A:13:PHE:HB3	1:A:56:TRP:CG	0.96	1.94	8	14
1:A:13:PHE:CG	1:A:56:TRP:HB2	0.95	1.96	12	14
1:A:39:ASP:HA	1:A:42:LYS:HD3	0.94	1.39	9	2
1:A:28:SER:HB2	1:A:32:LYS:HG2	0.93	1.38	3	2
1:A:15:LEU:HD13	1:A:39:ASP:HB3	0.93	1.40	9	8
1:A:23:LYS:HG2	1:A:56:TRP:CZ3	0.92	2.00	14	14
1:A:31:SER:HA	1:A:34:ILE:CD1	0.91	1.95	10	5
1:A:15:LEU:HD13	1:A:39:ASP:HB2	0.90	1.40	6	3
1:A:21:LEU:HD13	1:A:30:GLN:HB3	0.89	1.43	8	7
1:A:21:LEU:HD12	1:A:30:GLN:HB3	0.87	1.45	4	7
1:A:35:GLU:HA	1:A:40:PHE:CD2	0.87	2.04	7	10
1:A:10:ASN:HA	1:A:13:PHE:CD2	0.85	2.06	8	14
1:A:22:ASP:H	1:A:30:GLN:HG3	0.85	1.32	7	4
1:A:28:SER:HA	1:A:31:SER:OG	0.81	1.75	6	14
1:A:23:LYS:HZ2	1:A:53:PHE:HD2	0.79	1.20	13	3
1:A:27:TRP:CZ3	1:A:50:GLU:HA	0.79	2.13	7	14
1:A:27:TRP:CE2	1:A:50:GLU:HB3	0.78	2.13	15	14
1:A:11:ILE:O	1:A:15:LEU:HG	0.77	1.78	9	14
1:A:22:ASP:H	1:A:30:GLN:CG	0.76	1.93	10	4
1:A:16:PHE:O	1:A:21:LEU:HD23	0.76	1.81	5	7
1:A:16:PHE:CB	1:A:56:TRP:CZ3	0.75	2.70	9	14
1:A:56:TRP:HA	1:A:59:GLU:CB	0.75	2.12	7	13
1:A:34:ILE:HD12	1:A:35:GLU:H	0.74	1.42	14	3
1:A:12:PHE:CE1	1:A:43:ILE:HG12	0.73	2.17	8	5
1:A:23:LYS:HE3	1:A:56:TRP:HZ3	0.73	1.43	14	4
1:A:34:ILE:HB	1:A:40:PHE:HB2	0.73	1.59	12	5
1:A:21:LEU:HD12	1:A:30:GLN:CB	0.71	2.14	4	7
1:A:9:ARG:HA	1:A:52:LEU:HD22	0.71	1.62	12	11
1:A:13:PHE:CD2	1:A:56:TRP:HB2	0.70	2.22	10	11
1:A:23:LYS:NZ	1:A:23:LYS:HA	0.70	2.01	9	6
1:A:28:SER:O	1:A:32:LYS:HG2	0.69	1.88	15	7
1:A:49:ARG:O	1:A:52:LEU:HB2	0.69	1.87	1	14
1:A:31:SER:CA	1:A:34:ILE:HD11	0.67	2.14	13	4
1:A:56:TRP:CA	1:A:59:GLU:HB2	0.67	2.16	7	13
1:A:21:LEU:HB3	1:A:30:GLN:HB3	0.67	1.67	3	3
1:A:13:PHE:CD1	1:A:56:TRP:HB2	0.66	2.24	8	13
1:A:16:PHE:CE2	1:A:53:PHE:HB2	0.66	2.25	10	3
1:A:30:GLN:O	1:A:33:LYS:HB3	0.66	1.90	6	7
1:A:55:GLU:O	1:A:59:GLU:HB2	0.66	1.91	15	4
1:A:34:ILE:HD13	1:A:35:GLU:N	0.66	2.06	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:TRP:CE3	1:A:50:GLU:HB3	0.66	2.26	12	14
1:A:23:LYS:HG2	1:A:56:TRP:CE3	0.65	2.27	14	14
1:A:12:PHE:HE1	1:A:42:LYS:HB2	0.65	1.51	13	8
1:A:23:LYS:HA	1:A:23:LYS:CE	0.65	2.21	9	6
1:A:28:SER:O	1:A:32:LYS:HG3	0.64	1.92	14	2
1:A:21:LEU:HB2	1:A:23:LYS:NZ	0.63	2.08	10	4
1:A:16:PHE:CB	1:A:56:TRP:CH2	0.63	2.81	10	14
1:A:12:PHE:CE1	1:A:42:LYS:HB2	0.63	2.28	3	11
1:A:48:VAL:O	1:A:52:LEU:HG	0.63	1.94	3	12
1:A:24:PHE:HB3	1:A:57:CYS:SG	0.63	2.34	3	1
1:A:13:PHE:CB	1:A:56:TRP:CG	0.63	2.80	8	14
1:A:13:PHE:CG	1:A:56:TRP:CB	0.62	2.81	10	11
1:A:34:ILE:HD11	1:A:40:PHE:CD1	0.62	2.29	1	7
1:A:30:GLN:O	1:A:34:ILE:HG23	0.62	1.94	7	6
1:A:22:ASP:HB2	1:A:30:GLN:HE21	0.62	1.55	10	3
1:A:13:PHE:CA	1:A:16:PHE:HB2	0.62	2.25	10	14
1:A:34:ILE:CD1	1:A:35:GLU:H	0.61	2.08	13	3
1:A:21:LEU:CD1	1:A:30:GLN:HB3	0.61	2.23	8	12
1:A:27:TRP:HA	1:A:53:PHE:CZ	0.61	2.30	7	4
1:A:22:ASP:HB2	1:A:30:GLN:NE2	0.61	2.10	10	10
1:A:12:PHE:O	1:A:16:PHE:N	0.60	2.34	10	14
1:A:13:PHE:HA	1:A:56:TRP:CE3	0.60	2.32	9	14
1:A:23:LYS:CG	1:A:56:TRP:CZ3	0.60	2.83	10	14
1:A:16:PHE:HE1	1:A:34:ILE:HD13	0.60	1.55	6	7
1:A:38:PRO:HA	1:A:41:TYR:CZ	0.60	2.31	14	1
1:A:34:ILE:HD13	1:A:40:PHE:CG	0.60	2.31	14	3
1:A:50:GLU:O	1:A:53:PHE:HD1	0.59	1.80	15	9
1:A:51:SER:HA	1:A:54:GLU:OE2	0.59	1.98	11	2
1:A:30:GLN:O	1:A:33:LYS:HB2	0.59	1.98	12	3
1:A:24:PHE:HB2	1:A:57:CYS:SG	0.59	2.37	10	1
1:A:43:ILE:HD12	1:A:52:LEU:HD11	0.59	1.75	4	5
1:A:31:SER:HB2	1:A:40:PHE:CZ	0.58	2.33	3	4
1:A:29:LEU:O	1:A:33:LYS:HB2	0.58	1.97	6	1
1:A:13:PHE:HA	1:A:56:TRP:CD2	0.58	2.34	9	14
1:A:40:PHE:CD1	1:A:49:ARG:HD3	0.58	2.33	6	7
1:A:23:LYS:CE	1:A:56:TRP:HZ3	0.58	2.12	14	7
1:A:11:ILE:O	1:A:14:GLU:HB3	0.58	1.97	9	2
1:A:34:ILE:HD12	1:A:34:ILE:N	0.58	2.13	10	2
1:A:12:PHE:CG	1:A:52:LEU:HD23	0.58	2.32	1	2
1:A:50:GLU:O	1:A:53:PHE:HD2	0.58	1.80	4	2
1:A:15:LEU:CD1	1:A:39:ASP:HB2	0.58	2.26	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ILE:HG12	1:A:40:PHE:CD1	0.58	2.34	10	3
1:A:15:LEU:HD13	1:A:39:ASP:HA	0.58	1.76	5	1
1:A:23:LYS:NZ	1:A:30:GLN:HG3	0.58	2.13	4	5
1:A:13:PHE:N	1:A:13:PHE:CD1	0.57	2.72	3	3
1:A:23:LYS:HA	1:A:23:LYS:HZ3	0.57	1.58	12	4
1:A:23:LYS:CE	1:A:23:LYS:HA	0.57	2.29	4	4
1:A:49:ARG:HA	1:A:52:LEU:HD22	0.57	1.76	1	2
1:A:13:PHE:HA	1:A:16:PHE:HB2	0.57	1.76	10	14
1:A:13:PHE:CD1	1:A:13:PHE:N	0.56	2.74	4	11
1:A:23:LYS:HZ2	1:A:53:PHE:HD1	0.56	1.43	4	1
1:A:12:PHE:HB2	1:A:52:LEU:HD13	0.56	1.78	13	11
1:A:50:GLU:O	1:A:53:PHE:CD1	0.56	2.59	13	11
1:A:34:ILE:N	1:A:34:ILE:HD13	0.56	2.16	11	1
1:A:21:LEU:C	1:A:23:LYS:NZ	0.56	2.64	10	4
1:A:9:ARG:HD2	1:A:55:GLU:OE1	0.56	2.01	4	3
1:A:12:PHE:CG	1:A:52:LEU:HD13	0.55	2.37	6	3
1:A:49:ARG:HA	1:A:52:LEU:HD12	0.55	1.76	6	2
1:A:10:ASN:O	1:A:14:GLU:HB2	0.55	2.01	6	3
1:A:27:TRP:CE2	1:A:50:GLU:CB	0.55	2.88	15	14
1:A:23:LYS:CE	1:A:56:TRP:CZ3	0.55	2.90	14	4
1:A:26:THR:OG1	1:A:29:LEU:HB2	0.55	2.01	5	5
1:A:50:GLU:O	1:A:53:PHE:CD2	0.54	2.61	4	2
1:A:30:GLN:CD	1:A:30:GLN:N	0.54	2.66	10	2
1:A:23:LYS:HZ2	1:A:56:TRP:HH2	0.54	1.44	7	2
1:A:27:TRP:CE2	1:A:50:GLU:HG3	0.53	2.38	4	10
1:A:8:GLU:HB2	1:A:43:ILE:HD11	0.53	1.79	10	1
1:A:22:ASP:HB2	1:A:30:GLN:HE22	0.53	1.63	14	1
1:A:27:TRP:CE2	1:A:50:GLU:CG	0.53	2.91	7	14
1:A:34:ILE:CD1	1:A:35:GLU:N	0.53	2.72	13	4
1:A:16:PHE:HA	1:A:21:LEU:CD2	0.53	2.34	4	3
1:A:12:PHE:CB	1:A:52:LEU:HD13	0.53	2.34	6	3
1:A:35:GLU:HB3	1:A:40:PHE:CD2	0.53	2.39	5	3
1:A:32:LYS:HD3	1:A:32:LYS:C	0.53	2.28	4	3
1:A:35:GLU:HA	1:A:40:PHE:CE2	0.53	2.39	4	3
1:A:8:GLU:H	1:A:8:GLU:CD	0.52	2.11	13	8
1:A:8:GLU:O	1:A:11:ILE:HB	0.52	2.04	4	5
1:A:12:PHE:CD2	1:A:52:LEU:HD12	0.52	2.39	15	5
1:A:9:ARG:HD3	1:A:55:GLU:OE1	0.52	2.05	9	1
1:A:34:ILE:HD12	1:A:35:GLU:N	0.52	2.15	14	2
1:A:28:SER:C	1:A:30:GLN:N	0.52	2.66	6	14
1:A:9:ARG:NH2	1:A:55:GLU:HB3	0.52	2.20	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:PHE:CE1	1:A:49:ARG:HD3	0.52	2.40	13	4
1:A:43:ILE:HG22	1:A:45:ASP:H	0.51	1.64	8	2
1:A:8:GLU:HA	1:A:11:ILE:HD13	0.51	1.82	4	1
1:A:39:ASP:O	1:A:42:LYS:HB2	0.51	2.05	9	1
1:A:12:PHE:HB3	1:A:16:PHE:CZ	0.51	2.40	10	10
1:A:10:ASN:HA	1:A:13:PHE:CE2	0.51	2.40	9	10
1:A:23:LYS:HA	1:A:53:PHE:CE2	0.51	2.41	10	1
1:A:20:LYS:HB2	1:A:20:LYS:NZ	0.51	2.20	13	1
1:A:18:ARG:NE	1:A:18:ARG:HA	0.51	2.20	3	1
1:A:28:SER:O	1:A:32:LYS:N	0.50	2.44	1	7
1:A:27:TRP:HA	1:A:53:PHE:CE2	0.50	2.42	5	2
1:A:53:PHE:CD1	1:A:54:GLU:N	0.50	2.80	5	7
1:A:30:GLN:O	1:A:34:ILE:HG13	0.50	2.06	14	1
1:A:27:TRP:CZ2	1:A:50:GLU:HG3	0.50	2.42	7	5
1:A:46:ASP:OD1	1:A:49:ARG:HD2	0.50	2.07	7	2
1:A:33:LYS:HA	1:A:33:LYS:HE2	0.50	1.84	6	1
1:A:34:ILE:O	1:A:40:PHE:HB2	0.50	2.07	3	4
1:A:34:ILE:HD11	1:A:40:PHE:HD1	0.50	1.66	1	3
1:A:54:GLU:O	1:A:57:CYS:HB3	0.50	2.07	7	3
1:A:43:ILE:HG21	1:A:48:VAL:HB	0.50	1.84	8	1
1:A:31:SER:O	1:A:35:GLU:HB2	0.49	2.07	4	1
1:A:34:ILE:CD1	1:A:40:PHE:CD1	0.49	2.96	6	7
1:A:13:PHE:CB	1:A:56:TRP:HB2	0.49	2.35	8	3
1:A:44:ARG:HD3	1:A:44:ARG:H	0.49	1.68	8	1
1:A:9:ARG:HG3	1:A:13:PHE:CZ	0.49	2.43	9	1
1:A:32:LYS:HD2	1:A:32:LYS:C	0.49	2.33	9	1
1:A:23:LYS:CD	1:A:53:PHE:HD1	0.49	2.21	14	1
1:A:31:SER:O	1:A:35:GLU:HG2	0.49	2.08	9	2
1:A:21:LEU:HB3	1:A:30:GLN:CB	0.49	2.36	3	3
1:A:31:SER:C	1:A:33:LYS:N	0.48	2.71	3	7
1:A:21:LEU:HB3	1:A:30:GLN:CG	0.48	2.39	10	4
1:A:31:SER:HB2	1:A:40:PHE:CE1	0.48	2.43	7	2
1:A:32:LYS:HD3	1:A:33:LYS:N	0.48	2.24	4	1
1:A:21:LEU:HD12	1:A:30:GLN:CG	0.48	2.38	9	4
1:A:21:LEU:C	1:A:23:LYS:HZ1	0.48	2.14	10	1
1:A:22:ASP:N	1:A:30:GLN:HG3	0.48	2.15	1	1
1:A:50:GLU:CD	1:A:50:GLU:H	0.48	2.17	4	1
1:A:21:LEU:HD22	1:A:30:GLN:HA	0.48	1.84	7	1
1:A:45:ASP:HB2	1:A:48:VAL:HG23	0.48	1.85	8	1
1:A:39:ASP:O	1:A:42:LYS:HG2	0.48	2.09	10	1
1:A:21:LEU:HD22	1:A:30:GLN:CB	0.48	2.38	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:PHE:CD1	1:A:54:GLU:HG2	0.48	2.44	12	2
1:A:49:ARG:HA	1:A:52:LEU:CD1	0.48	2.39	4	3
1:A:56:TRP:C	1:A:59:GLU:HB2	0.48	2.34	13	4
1:A:21:LEU:HD13	1:A:30:GLN:CB	0.47	2.34	1	4
1:A:28:SER:O	1:A:29:LEU:C	0.47	2.54	11	12
1:A:21:LEU:CB	1:A:30:GLN:HB3	0.47	2.38	3	2
1:A:22:ASP:O	1:A:30:GLN:HG2	0.47	2.10	1	1
1:A:23:LYS:HE3	1:A:56:TRP:CZ3	0.47	2.33	14	1
1:A:30:GLN:N	1:A:30:GLN:CD	0.47	2.73	7	5
1:A:15:LEU:HD13	1:A:39:ASP:CB	0.47	2.32	7	2
1:A:32:LYS:NZ	1:A:32:LYS:HB2	0.47	2.25	12	1
1:A:9:ARG:HB2	1:A:13:PHE:CZ	0.47	2.45	7	1
1:A:12:PHE:HB2	1:A:52:LEU:HG	0.47	1.87	8	1
1:A:44:ARG:HG3	1:A:45:ASP:N	0.47	2.25	15	1
1:A:29:LEU:O	1:A:33:LYS:HE2	0.46	2.10	1	1
1:A:7:ASP:O	1:A:11:ILE:HG12	0.46	2.10	9	1
1:A:53:PHE:O	1:A:57:CYS:HB2	0.46	2.11	7	4
1:A:16:PHE:C	1:A:21:LEU:HD23	0.46	2.36	4	5
1:A:23:LYS:HZ1	1:A:30:GLN:HG3	0.46	1.71	9	2
1:A:12:PHE:O	1:A:16:PHE:CG	0.46	2.68	4	12
1:A:33:LYS:C	1:A:33:LYS:HD2	0.46	2.35	15	1
1:A:13:PHE:C	1:A:16:PHE:HB2	0.46	2.36	3	10
1:A:12:PHE:CG	1:A:52:LEU:CD1	0.46	2.99	9	5
1:A:12:PHE:CE1	1:A:43:ILE:HG13	0.46	2.46	5	1
1:A:9:ARG:HA	1:A:52:LEU:CD2	0.45	2.41	6	1
1:A:9:ARG:HB2	1:A:52:LEU:HD22	0.45	1.87	9	1
1:A:30:GLN:O	1:A:33:LYS:HG2	0.45	2.12	9	1
1:A:31:SER:C	1:A:33:LYS:H	0.45	2.19	3	3
1:A:13:PHE:O	1:A:17:ASP:N	0.45	2.49	13	7
1:A:31:SER:HA	1:A:34:ILE:HG12	0.45	1.89	15	2
1:A:13:PHE:HB3	1:A:56:TRP:CB	0.45	2.41	8	4
1:A:9:ARG:HG3	1:A:10:ASN:N	0.45	2.27	4	7
1:A:13:PHE:CA	1:A:56:TRP:CD2	0.45	2.99	10	11
1:A:31:SER:CA	1:A:34:ILE:CD1	0.45	2.84	10	1
1:A:21:LEU:HD22	1:A:30:GLN:HB3	0.44	1.87	12	1
1:A:8:GLU:HA	1:A:11:ILE:HD12	0.44	1.90	5	1
1:A:13:PHE:CE1	1:A:52:LEU:O	0.44	2.71	15	10
1:A:23:LYS:O	1:A:23:LYS:HD3	0.44	2.12	11	1
1:A:9:ARG:CA	1:A:52:LEU:HD22	0.44	2.40	15	1
1:A:35:GLU:CA	1:A:40:PHE:CD2	0.44	3.01	6	1
1:A:42:LYS:HA	1:A:42:LYS:HE2	0.44	1.90	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:LYS:CG	1:A:56:TRP:CE3	0.43	3.00	8	2
1:A:34:ILE:HD13	1:A:40:PHE:CD2	0.43	2.48	13	2
1:A:28:SER:O	1:A:32:LYS:HD2	0.43	2.14	4	1
1:A:29:LEU:O	1:A:33:LYS:HB3	0.43	2.13	15	1
1:A:27:TRP:CH2	1:A:50:GLU:HA	0.43	2.47	10	3
1:A:39:ASP:HA	1:A:42:LYS:HG2	0.43	1.89	3	1
1:A:30:GLN:N	1:A:30:GLN:OE1	0.43	2.50	3	2
1:A:30:GLN:CD	1:A:30:GLN:H	0.43	2.21	10	1
1:A:16:PHE:HA	1:A:21:LEU:HD23	0.43	1.90	15	2
1:A:34:ILE:O	1:A:37:ASP:HB2	0.43	2.13	11	3
1:A:21:LEU:CG	1:A:30:GLN:HB3	0.42	2.44	1	1
1:A:22:ASP:HB3	1:A:25:SER:OG	0.42	2.14	6	1
1:A:37:ASP:HB2	1:A:39:ASP:OD1	0.42	2.14	6	1
1:A:23:LYS:HD2	1:A:53:PHE:O	0.42	2.14	11	1
1:A:23:LYS:NZ	1:A:53:PHE:HD2	0.42	2.12	11	3
1:A:16:PHE:CE1	1:A:34:ILE:HD13	0.42	2.48	3	1
1:A:34:ILE:CD1	1:A:34:ILE:N	0.42	2.83	10	1
1:A:50:GLU:OE1	1:A:50:GLU:N	0.42	2.52	14	2
1:A:32:LYS:HA	1:A:35:GLU:HG2	0.42	1.90	6	1
1:A:18:ARG:HA	1:A:18:ARG:CZ	0.42	2.45	3	1
1:A:12:PHE:HB3	1:A:16:PHE:CE2	0.42	2.50	7	3
1:A:53:PHE:HD1	1:A:54:GLU:HG2	0.42	1.75	8	1
1:A:35:GLU:HA	1:A:40:PHE:HD2	0.41	1.72	6	1
1:A:23:LYS:HE2	1:A:56:TRP:CZ3	0.41	2.50	8	1
1:A:31:SER:HA	1:A:34:ILE:HD12	0.41	1.85	10	1
1:A:57:CYS:SG	1:A:58:GLY:N	0.41	2.94	1	1
1:A:22:ASP:CB	1:A:25:SER:HB2	0.41	2.45	10	1
1:A:22:ASP:HB3	1:A:25:SER:HB2	0.41	1.92	10	1
1:A:23:LYS:NZ	1:A:56:TRP:CH2	0.41	2.79	10	1
1:A:9:ARG:HG2	1:A:10:ASN:ND2	0.41	2.31	9	1
1:A:22:ASP:H	1:A:30:GLN:HG2	0.41	1.72	10	1
1:A:27:TRP:O	1:A:30:GLN:HB2	0.41	2.16	6	1
1:A:34:ILE:HD12	1:A:34:ILE:H	0.41	1.77	10	1
1:A:30:GLN:O	1:A:33:LYS:HG3	0.41	2.15	15	1
1:A:34:ILE:HB	1:A:39:ASP:HB3	0.41	1.93	15	1
1:A:35:GLU:C	1:A:37:ASP:H	0.40	2.24	10	1
1:A:23:LYS:HG3	1:A:57:CYS:CA	0.40	2.46	15	1
1:A:13:PHE:CB	1:A:56:TRP:CB	0.40	3.00	14	1
1:A:20:LYS:HB3	1:A:20:LYS:NZ	0.40	2.31	6	1
1:A:27:TRP:CG	1:A:31:SER:HG	0.40	2.34	12	1
1:A:15:LEU:CD1	1:A:39:ASP:HA	0.40	2.46	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:GLU:HA	1:A:40:PHE:CB	0.40	2.47	5	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	52/59 (88%)	46±2 (88±4%)	3±1 (7±3%)	2±1 (4±2%)	4	29
All	All	773/885 (87%)	689 (89%)	52 (7%)	32 (4%)	4	29

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	7	ASP	13
1	A	35	GLU	9
1	A	20	LYS	5
1	A	25	SER	4
1	A	36	ASN	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	52/55 (95%)	41±2 (80±4%)	10±1 (20±3%)	3	33
All	All	776/825 (94%)	621 (80%)	155 (20%)	3	33

All 21 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	13	PHE	15
1	A	23	LYS	15
1	A	26	THR	15
1	A	50	GLU	15
1	A	8	GLU	14
1	A	53	PHE	14
1	A	59	GLU	9
1	A	40	PHE	7
1	A	21	LEU	7
1	A	32	LYS	6
1	A	34	ILE	6
1	A	20	LYS	4
1	A	35	GLU	4
1	A	33	LYS	4
1	A	30	GLN	3
1	A	52	LEU	3
1	A	54	GLU	3
1	A	36	ASN	3
1	A	14	GLU	3
1	A	29	LEU	3
1	A	47	THR	2

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 oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	3-A	2
1	7-A	2
1	9-A	2
1	15-A	2
1	1-A	1
1	4-A	1
1	5-A	1
1	8-A	1
1	11-A	1
1	12-A	1
1	13-A	1
1	14-A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	7:ASP	C	8:GLU	N	1.20
3	A	52:LEU	C	53:PHE	N	1.20
4	A	52:LEU	C	53:PHE	N	1.20
5	A	52:LEU	C	53:PHE	N	1.20
7	A	7:ASP	C	8:GLU	N	1.20
7	A	52:LEU	C	53:PHE	N	1.20
8	A	7:ASP	C	8:GLU	N	1.20
9	A	7:ASP	C	8:GLU	N	1.20
9	A	52:LEU	C	53:PHE	N	1.20
11	A	7:ASP	C	8:GLU	N	1.20
12	A	7:ASP	C	8:GLU	N	1.20
13	A	7:ASP	C	8:GLU	N	1.20
14	A	7:ASP	C	8:GLU	N	1.20
15	A	7:ASP	C	8:GLU	N	1.20
15	A	52:LEU	C	53:PHE	N	1.20
3	A	7:ASP	C	8:GLU	N	1.19

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 48% 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

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	397
Number of shifts mapped to atoms	385
Number of unparsed shifts	0
Number of shifts with mapping errors	12
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

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

- No matching atom found in the structure. All 12 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	ALA	H	8.595	0.02	1
1	A	2	ALA	HA	4.115	0.02	1
1	A	2	ALA	HB1	1.242	0.005	1
1	A	2	ALA	HB2	1.242	0.005	1
1	A	2	ALA	HB3	1.242	0.005	1
1	A	3	MET	H	8.439	0.009	1
1	A	3	MET	HA	4.325	0.02	1
1	A	3	MET	HB2	1.932	0.003	.
1	A	3	MET	HB3	1.858	0.005	.
1	A	3	MET	HG2	2.431	0.001	.
1	A	3	MET	HG3	2.359	0.002	.
1	A	4	GLY	H	8.086	0.016	1

7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

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 48%, i.e. 367 atoms were assigned a chemical shift out of a possible 771. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	105/264 (40%)	105/106 (99%)	0/106 (0%)	0/52 (0%)
Sidechain	218/405 (54%)	218/254 (86%)	0/131 (0%)	0/20 (0%)
Aromatic	44/102 (43%)	44/50 (88%)	0/50 (0%)	0/2 (0%)
Overall	367/771 (48%)	367/410 (90%)	0/287 (0%)	0/74 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 48%, i.e. 382 atoms were assigned a chemical shift out of a possible 798. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	109/274 (40%)	109/110 (99%)	0/110 (0%)	0/54 (0%)
Sidechain	229/422 (54%)	229/265 (86%)	0/137 (0%)	0/20 (0%)
Aromatic	44/102 (43%)	44/50 (88%)	0/50 (0%)	0/2 (0%)
Overall	382/798 (48%)	382/425 (90%)	0/297 (0%)	0/76 (0%)

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	31	SER	HB3	1.19	2.49 – 5.20	-9.8
1	A	23	LYS	HE3	1.24	1.92 – 3.89	-8.5
1	A	23	LYS	HE2	1.73	1.95 – 3.88	-6.1
1	A	31	SER	HB2	2.38	2.61 – 5.13	-5.9
1	A	16	PHE	HB3	0.82	1.03 – 4.85	-5.5

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:

