wwPDB NMR Structure Validation Summary Report

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PDB ID	:	5LCI
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Title	:	Solution structure of BOLA1 from Homo sapiens
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This is a wwPDB NMR Structure Validation Summary 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:

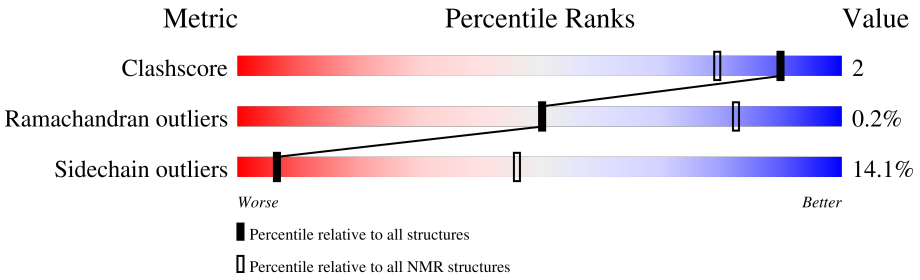
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 86%.

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	123	60% 10% • 28%

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *medoid*.

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:31-A:118 (88)	1.13	2

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 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1342 atoms, of which 669 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BolA-like protein 1.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	88	1342	419	669	129	125	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	-	expression tag	UNP Q9Y3E2
A	16	ILE	-	expression tag	UNP Q9Y3E2
A	17	ASP	-	expression tag	UNP Q9Y3E2
A	18	PRO	-	expression tag	UNP Q9Y3E2
A	19	PHE	-	expression tag	UNP Q9Y3E2
A	20	THR	-	expression tag	UNP Q9Y3E2

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: BolA-like protein 1

Chain A:

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 2. Colouring as in section 4.1 above.

- Molecule 1: BolA-like protein 1

Chain A:

5 Refinement protocol and experimental data overview

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

Of the 40 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
Amber	refinement	
UNIO	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1369
Number of shifts mapped to atoms	1022
Number of unparsed shifts	0
Number of shifts with mapping errors	347
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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	0.68±0.01	0±0/688 (0.0± 0.0%)	1.31±0.03	8±2/935 (0.8± 0.2%)
All	All	0.68	0/13760 (0.0%)	1.31	155/18700 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.8±0.6
All	All	0	35

There are no bond-length outliers.

5 of 23 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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	37	ARG	NE-CZ-NH1	11.03	125.81	120.30	15	18
1	A	85	ARG	NE-CZ-NH1	10.01	125.31	120.30	12	12
1	A	76	ARG	NE-CZ-NH1	9.60	125.10	120.30	18	16
1	A	69	ARG	NE-CZ-NH1	9.51	125.05	120.30	5	15
1	A	52	ARG	NE-CZ-NH1	9.24	124.92	120.30	11	16

There are no chirality outliers.

5 of 12 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	48	VAL	Peptide	10
1	A	117	ASN	Peptide	5
1	A	46	PRO	Peptide	4

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	66	THR	Peptide	4
1	A	106	ILE	Peptide	2

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	673	669	669	2±1
All	All	13460	13380	13380	45

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 2.

5 of 11 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:HIS:CD2	1:A:103:ALA:HB3	0.58	2.34	9	20
1:A:48:VAL:HG22	1:A:73:VAL:HB	0.58	1.74	5	8
1:A:48:VAL:HG11	1:A:114:TRP:CE2	0.49	2.41	18	3
1:A:48:VAL:CG2	1:A:73:VAL:HB	0.47	2.39	3	6
1:A:73:VAL:HG21	1:A:114:TRP:CE3	0.45	2.47	9	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	86/123 (70%)	80±1 (93±2%)	6±1 (6±2%)	0±0 (0±0%)	50	82
All	All	1720/2460 (70%)	1605 (93%)	111 (6%)	4 (0%)	50	82

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occur-

rence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	55	SER	1
1	A	98	GLY	1
1	A	117	ASN	1
1	A	46	PRO	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	70/95 (74%)	60±2 (86±3%)	10±2 (14±3%)	6 46
All	All	1400/1900 (74%)	1203 (86%)	197 (14%)	6 46

5 of 38 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	67	HIS	20
1	A	80	LEU	13
1	A	53	ASN	11
1	A	69	ARG	10
1	A	49	LEU	10

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

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 86% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *BOLA1_NMRv3.str*

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	1369
Number of shifts mapped to atoms	1022
Number of unparsed shifts	0
Number of shifts with mapping errors	347
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. First 5 (of 347) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	16	ILE	C	174.726	0.300	1
1	A	16	ILE	CA	59.836	0.300	1
1	A	16	ILE	CB	37.905	0.300	1
1	A	16	ILE	CG1	25.858	0.300	1
1	A	16	ILE	CG2	16.071	0.300	1
1	A	16	ILE	CD1	11.706	0.300	1
1	A	16	ILE	HA	4.057	0.020	1
1	A	16	ILE	HB	1.675	0.020	1
1	A	16	ILE	HG12	1.306	0.020	2
1	A	16	ILE	HG13	1.04	0.020	2
1	A	16	ILE	HG21	0.748	0.020	1
1	A	16	ILE	HG22	0.748	0.020	1
1	A	16	ILE	HG23	0.748	0.020	1
1	A	16	ILE	HD11	0.73	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	16	ILE	HD12	0.73	0.020	1
1	A	16	ILE	HD13	0.73	0.020	1
1	A	17	ASP	C	173.934	0.300	1
1	A	17	ASP	CA	50.978	0.300	1
1	A	17	ASP	CB	40.278	0.300	1
1	A	17	ASP	H	8.4	0.020	1
1	A	17	ASP	HA	4.774	0.020	1
1	A	17	ASP	HB2	2.669	0.020	2
1	A	17	ASP	HB3	2.471	0.020	2
1	A	17	ASP	N	126.24	0.300	1
1	A	18	PRO	C	176.142	0.300	1
1	A	18	PRO	CA	62.616	0.300	1
1	A	18	PRO	CB	30.783	0.300	1
1	A	18	PRO	CG	25.475	0.300	1
1	A	18	PRO	CD	49.848	0.300	1
1	A	18	PRO	HA	4.196	0.020	1
1	A	18	PRO	HB2	1.508	0.020	2
1	A	18	PRO	HB3	2.018	0.020	2
1	A	18	PRO	HG2	1.804	0.020	2
1	A	18	PRO	HG3	1.634	0.020	2
1	A	18	PRO	HD2	3.774	0.020	2
1	A	18	PRO	HD3	3.666	0.020	2
1	A	19	PHE	C	175.435	0.300	1
1	A	19	PHE	CA	57.284	0.300	1
1	A	19	PHE	CB	37.76	0.300	1
1	A	19	PHE	H	8.208	0.020	1
1	A	19	PHE	HA	4.483	0.020	1
1	A	19	PHE	HB2	3.084	0.020	2
1	A	19	PHE	HB3	3.022	0.020	2
1	A	19	PHE	HD1	7.16	0.020	1
1	A	19	PHE	HD2	7.16	0.020	1
1	A	19	PHE	N	118.391	0.300	1
1	A	20	THR	C	173.551	0.300	1
1	A	20	THR	CA	61.056	0.300	1
1	A	20	THR	CB	68.842	0.300	1
1	A	20	THR	CG2	20.49	0.300	1
1	A	20	THR	H	7.75	0.020	1
1	A	20	THR	HA	4.193	0.020	1
1	A	20	THR	HB	4.113	0.020	1
1	A	20	THR	HG21	1.098	0.020	1
1	A	20	THR	HG22	1.098	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	20	THR	HG23	1.098	0.020	1
1	A	20	THR	N	114.115	0.300	1
1	A	21	GLN	C	175.444	0.300	1
1	A	21	GLN	CA	55.171	0.300	1
1	A	21	GLN	CB	28.307	0.300	1
1	A	21	GLN	CG	32.329	0.300	1
1	A	21	GLN	H	8.164	0.020	1
1	A	21	GLN	HA	4.208	0.020	1
1	A	21	GLN	HB2	1.934	0.020	1
1	A	21	GLN	HB3	1.934	0.020	1
1	A	21	GLN	HG2	2.258	0.020	2
1	A	21	GLN	HG3	2.084	0.020	2
1	A	21	GLN	HE21	7.225	0.020	1
1	A	21	GLN	HE22	6.906	0.020	1
1	A	21	GLN	N	122.223	0.300	1
1	A	21	GLN	NE2	110.517	0.300	1
1	A	22	GLY	C	173.2	0.300	1
1	A	22	GLY	CA	44.198	0.300	1
1	A	22	GLY	H	8.323	0.020	1
1	A	22	GLY	HA2	3.872	0.020	2
1	A	22	GLY	HA3	3.835	0.020	2
1	A	22	GLY	N	109.739	0.300	1
1	A	23	SER	C	173.602	0.300	1
1	A	23	SER	CA	57.28	0.300	1
1	A	23	SER	CB	62.845	0.300	1
1	A	23	SER	H	8.163	0.020	1
1	A	23	SER	HA	4.361	0.020	1
1	A	23	SER	HB2	3.764	0.020	2
1	A	23	SER	HB3	3.674	0.020	2
1	A	23	SER	N	115.46	0.300	1
1	A	24	ALA	C	177.285	0.300	1
1	A	24	ALA	CA	51.814	0.300	1
1	A	24	ALA	CB	17.928	0.300	1
1	A	24	ALA	H	8.361	0.020	1
1	A	24	ALA	HA	4.229	0.020	1
1	A	24	ALA	HB1	1.283	0.020	1
1	A	24	ALA	HB2	1.283	0.020	1
1	A	24	ALA	HB3	1.283	0.020	1
1	A	24	ALA	N	125.644	0.300	1
1	A	25	GLY	C	173.43	0.300	1
1	A	25	GLY	CA	44.217	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	25	GLY	H	8.273	0.020	1
1	A	25	GLY	HA2	3.868	0.020	1
1	A	25	GLY	HA3	3.868	0.020	1
1	A	25	GLY	N	107.826	0.300	1
1	A	26	SER	C	174.147	0.300	1
1	A	26	SER	CA	57.633	0.300	1
1	A	26	SER	CB	62.845	0.300	1
1	A	26	SER	H	8.211	0.020	1
1	A	26	SER	HA	4.349	0.020	1
1	A	26	SER	HB2	3.841	0.020	2
1	A	26	SER	HB3	3.8	0.020	2
1	A	26	SER	N	115.46	0.300	1
1	A	27	GLY	C	172.603	0.300	1
1	A	27	GLY	CA	44.194	0.300	1
1	A	27	GLY	H	8.414	0.020	1
1	A	27	GLY	HA2	3.884	0.020	2
1	A	27	GLY	HA3	3.832	0.020	2
1	A	27	GLY	N	110.804	0.300	1
1	A	28	ALA	C	176.295	0.300	1
1	A	28	ALA	CA	51.227	0.300	1
1	A	28	ALA	CB	18.371	0.300	1
1	A	28	ALA	H	8.011	0.020	1
1	A	28	ALA	HA	4.269	0.020	1
1	A	28	ALA	HB1	1.223	0.020	1
1	A	28	ALA	HB2	1.223	0.020	1
1	A	28	ALA	HB3	1.223	0.020	1
1	A	28	ALA	N	123.552	0.300	1
1	A	29	ILE	C	175.432	0.300	1
1	A	29	ILE	CA	60.032	0.300	1
1	A	29	ILE	CB	38.049	0.300	1
1	A	29	ILE	CG1	25.514	0.300	1
1	A	29	ILE	CG2	16.077	0.300	1
1	A	29	ILE	CD1	11.702	0.300	1
1	A	29	ILE	H	8.023	0.020	1
1	A	29	ILE	HA	4.078	0.020	1
1	A	29	ILE	HB	1.685	0.020	1
1	A	29	ILE	HG12	1.12	0.020	2
1	A	29	ILE	HG13	1.417	0.020	2
1	A	29	ILE	HG21	0.863	0.020	1
1	A	29	ILE	HG22	0.863	0.020	1
1	A	29	ILE	HG23	0.863	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	29	ILE	HD11	0.725	0.020	1
1	A	29	ILE	HD12	0.725	0.020	1
1	A	29	ILE	HD13	0.725	0.020	1
1	A	29	ILE	N	120.372	0.300	1
1	A	30	GLY	C	170.367	0.300	1
1	A	30	GLY	CA	44.199	0.300	1
1	A	30	GLY	H	8.237	0.020	1
1	A	30	GLY	HA2	3.845	0.020	1
1	A	30	GLY	HA3	3.845	0.020	1
1	A	30	GLY	N	114.98	0.300	1
1	A	119	GLN	C	175.022	0.300	1
1	A	119	GLN	CA	54.787	0.300	1
1	A	119	GLN	CB	28.046	0.300	1
1	A	119	GLN	CG	32.341	0.300	1
1	A	119	GLN	H	7.86	0.020	1
1	A	119	GLN	HA	4.107	0.020	1
1	A	119	GLN	HB2	1.863	0.020	1
1	A	119	GLN	HB3	1.863	0.020	1
1	A	119	GLN	HG2	2.27	0.020	2
1	A	119	GLN	HG3	2.186	0.020	2
1	A	119	GLN	HE21	7.391	0.020	1
1	A	119	GLN	HE22	6.703	0.020	1
1	A	119	GLN	N	120.572	0.300	1
1	A	119	GLN	NE2	112.341	0.300	1
1	A	120	LEU	C	176.022	0.300	1
1	A	120	LEU	CA	54.009	0.300	1
1	A	120	LEU	CB	41.436	0.300	1
1	A	120	LEU	CG	25.464	0.300	1
1	A	120	LEU	CD1	23.617	0.300	1
1	A	120	LEU	CD2	22.338	0.300	1
1	A	120	LEU	H	8.146	0.020	1
1	A	120	LEU	HA	4.264	0.020	1
1	A	120	LEU	HB2	1.554	0.020	2
1	A	120	LEU	HB3	1.453	0.020	2
1	A	120	LEU	HG	1.525	0.020	1
1	A	120	LEU	HD11	0.808	0.020	1
1	A	120	LEU	HD12	0.808	0.020	1
1	A	120	LEU	HD13	0.808	0.020	1
1	A	120	LEU	HD21	0.746	0.020	1
1	A	120	LEU	HD22	0.746	0.020	1
1	A	120	LEU	HD23	0.746	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	120	LEU	N	123.345	0.300	1
1	A	121	ASP	C	175.439	0.300	1
1	A	121	ASP	CA	53.333	0.300	1
1	A	121	ASP	CB	40.029	0.300	1
1	A	121	ASP	H	8.348	0.020	1
1	A	121	ASP	HA	4.505	0.020	1
1	A	121	ASP	HB2	2.607	0.020	2
1	A	121	ASP	HB3	2.507	0.020	2
1	A	121	ASP	N	121.556	0.300	1
1	A	122	THR	C	173.595	0.300	1
1	A	122	THR	CA	60.451	0.300	1
1	A	122	THR	CB	68.313	0.300	1
1	A	122	THR	CG2	20.477	0.300	1
1	A	122	THR	H	7.997	0.020	1
1	A	122	THR	HA	4.2	0.020	1
1	A	122	THR	HB	4.147	0.020	1
1	A	122	THR	HG21	1.089	0.020	1
1	A	122	THR	HG22	1.089	0.020	1
1	A	122	THR	HG23	1.089	0.020	1
1	A	122	THR	N	113.351	0.300	1
1	A	123	SER	C	170.899	0.300	1
1	A	123	SER	CA	55.91	0.300	1
1	A	123	SER	CB	62.004	0.300	1
1	A	123	SER	H	8.209	0.020	1
1	A	123	SER	HA	4.59	0.020	1
1	A	123	SER	HB2	3.678	0.020	1
1	A	123	SER	HB3	3.678	0.020	1
1	A	123	SER	N	119.459	0.300	1
1	A	125	PRO	C	175.629	0.300	1
1	A	125	PRO	CA	62.057	0.300	1
1	A	125	PRO	CB	30.865	0.300	1
1	A	125	PRO	CG	26.103	0.300	1
1	A	125	PRO	CD	49.206	0.300	1
1	A	125	PRO	HA	4.286	0.020	1
1	A	125	PRO	HB2	2.137	0.020	2
1	A	125	PRO	HB3	1.736	0.020	2
1	A	125	PRO	HG2	1.907	0.020	1
1	A	125	PRO	HG3	1.907	0.020	1
1	A	125	PRO	HD2	3.694	0.020	2
1	A	125	PRO	HD3	3.552	0.020	2
1	A	126	CYS	C	173.792	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	126	CYS	CA	57.275	0.300	1
1	A	126	CYS	CB	26.7	0.300	1
1	A	126	CYS	H	8.365	0.020	1
1	A	126	CYS	HA	4.362	0.020	1
1	A	126	CYS	HB2	2.745	0.020	1
1	A	126	CYS	HB3	2.745	0.020	1
1	A	126	CYS	N	119.277	0.300	1
1	A	127	LEU	C	176.782	0.300	1
1	A	127	LEU	CA	54.293	0.300	1
1	A	127	LEU	CB	41.207	0.300	1
1	A	127	LEU	CG	25.464	0.300	1
1	A	127	LEU	CD1	23.581	0.300	1
1	A	127	LEU	CD2	22.351	0.300	1
1	A	127	LEU	H	8.368	0.020	1
1	A	127	LEU	HA	4.235	0.020	1
1	A	127	LEU	HB2	1.487	0.020	1
1	A	127	LEU	HB3	1.487	0.020	1
1	A	127	LEU	HG	1.525	0.020	1
1	A	127	LEU	HD11	0.808	0.020	1
1	A	127	LEU	HD12	0.808	0.020	1
1	A	127	LEU	HD13	0.808	0.020	1
1	A	127	LEU	HD21	0.74	0.020	1
1	A	127	LEU	HD22	0.74	0.020	1
1	A	127	LEU	HD23	0.74	0.020	1
1	A	127	LEU	N	125.444	0.300	1
1	A	128	GLY	C	173.635	0.300	1
1	A	128	GLY	CA	44.284	0.300	1
1	A	128	GLY	H	8.381	0.020	1
1	A	128	GLY	HA2	3.81	0.020	1
1	A	128	GLY	HA3	3.81	0.020	1
1	A	128	GLY	N	109.598	0.300	1
1	A	129	GLY	C	172.969	0.300	1
1	A	129	GLY	CA	44.187	0.300	1
1	A	129	GLY	H	8.174	0.020	1
1	A	129	GLY	HA2	3.81	0.020	1
1	A	129	GLY	HA3	3.81	0.020	1
1	A	129	GLY	N	108.342	0.300	1
1	A	130	ASN	C	174.272	0.300	1
1	A	130	ASN	CA	52.118	0.300	1
1	A	130	ASN	CB	37.768	0.300	1
1	A	130	ASN	H	8.277	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	130	ASN	HA	4.55	0.020	1
1	A	130	ASN	HB2	2.709	0.020	2
1	A	130	ASN	HB3	2.652	0.020	2
1	A	130	ASN	HD21	6.83	0.020	1
1	A	130	ASN	HD22	7.508	0.020	1
1	A	130	ASN	N	118.356	0.300	1
1	A	130	ASN	ND2	112.619	0.300	1
1	A	131	LYS	C	175.552	0.300	1
1	A	131	LYS	CA	55.559	0.300	1
1	A	131	LYS	CB	31.861	0.300	1
1	A	131	LYS	CG	23.601	0.300	1
1	A	131	LYS	CD	27.9	0.300	1
1	A	131	LYS	CE	41.093	0.300	1
1	A	131	LYS	H	8.223	0.020	1
1	A	131	LYS	HA	4.144	0.020	1
1	A	131	LYS	HB2	1.725	0.020	2
1	A	131	LYS	HB3	1.656	0.020	2
1	A	131	LYS	HG2	1.335	0.020	2
1	A	131	LYS	HG3	1.288	0.020	2
1	A	131	LYS	HD2	1.562	0.020	1
1	A	131	LYS	HD3	1.562	0.020	1
1	A	131	LYS	HE2	2.876	0.020	1
1	A	131	LYS	HE3	2.876	0.020	1
1	A	131	LYS	N	121.335	0.300	1
1	A	132	LYS	C	175.666	0.300	1
1	A	132	LYS	CA	55.477	0.300	1
1	A	132	LYS	CB	31.904	0.300	1
1	A	132	LYS	CG	23.594	0.300	1
1	A	132	LYS	CD	27.935	0.300	1
1	A	132	LYS	CE	41.089	0.300	1
1	A	132	LYS	H	8.257	0.020	1
1	A	132	LYS	HA	4.216	0.020	1
1	A	132	LYS	HB2	1.652	0.020	1
1	A	132	LYS	HB3	1.652	0.020	1
1	A	132	LYS	HG2	1.562	0.020	1
1	A	132	LYS	HG3	1.562	0.020	1
1	A	132	LYS	HD2	1.562	0.020	1
1	A	132	LYS	HD3	1.562	0.020	1
1	A	132	LYS	HE2	2.874	0.020	1
1	A	132	LYS	HE3	2.874	0.020	1
1	A	132	LYS	N	122.264	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	133	THR	C	173.435	0.300	1
1	A	133	THR	CA	60.729	0.300	1
1	A	133	THR	CB	68.602	0.300	1
1	A	133	THR	CG2	20.781	0.300	1
1	A	133	THR	H	8.096	0.020	1
1	A	133	THR	HA	4.176	0.020	1
1	A	133	THR	HB	4.074	0.020	1
1	A	133	THR	HG21	1.09	0.020	1
1	A	133	THR	HG22	1.09	0.020	1
1	A	133	THR	HG23	1.09	0.020	1
1	A	133	THR	N	115.813	0.300	1
1	A	134	LEU	C	176.728	0.300	1
1	A	134	LEU	CA	54.384	0.300	1
1	A	134	LEU	CB	41.221	0.300	1
1	A	134	LEU	CG	25.479	0.300	1
1	A	134	LEU	CD1	23.632	0.300	1
1	A	134	LEU	CD2	22.349	0.300	1
1	A	134	LEU	H	8.258	0.020	1
1	A	134	LEU	HA	4.212	0.020	1
1	A	134	LEU	HB2	1.499	0.020	2
1	A	134	LEU	HB3	1.443	0.020	2
1	A	134	LEU	HG	1.51	0.020	1
1	A	134	LEU	HD11	1.517	0.020	1
1	A	134	LEU	HD12	1.517	0.020	1
1	A	134	LEU	HD13	1.517	0.020	1
1	A	134	LEU	HD21	0.788	0.020	1
1	A	134	LEU	HD22	0.788	0.020	1
1	A	134	LEU	HD23	0.788	0.020	1
1	A	134	LEU	N	124.632	0.300	1
1	A	135	GLY	C	172.846	0.300	1
1	A	135	GLY	CA	44.086	0.300	1
1	A	135	GLY	H	8.342	0.020	1
1	A	135	GLY	HA2	3.831	0.020	1
1	A	135	GLY	HA3	3.831	0.020	1
1	A	135	GLY	N	109.662	0.300	1
1	A	136	THR	C	171.187	0.300	1
1	A	136	THR	CA	58.49	0.300	1
1	A	136	THR	CB	68.748	0.300	1
1	A	136	THR	CG2	19.848	0.300	1
1	A	136	THR	H	7.877	0.020	1
1	A	136	THR	HA	4.507	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	136	THR	HB	4.04	0.020	1
1	A	136	THR	HG21	1.139	0.020	1
1	A	136	THR	HG22	1.139	0.020	1
1	A	136	THR	HG23	1.139	0.020	1
1	A	136	THR	N	115.983	0.300	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
$^{13}C_{\alpha}$	118	1.00 ± 0.18	Should be applied
$^{13}C_{\beta}$	105	1.25 ± 0.13	Should be applied
$^{13}C'$	116	0.92 ± 0.13	Should be applied
^{15}N	109	0.33 ± 0.35	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 86%, i.e. 1022 atoms were assigned a chemical shift out of a possible 1192. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	422/432 (98%)	172/175 (98%)	170/176 (97%)	80/81 (99%)
Sidechain	564/688 (82%)	386/450 (86%)	175/208 (84%)	3/30 (10%)
Aromatic	36/72 (50%)	25/36 (69%)	0/25 (0%)	11/11 (100%)
Overall	1022/1192 (86%)	583/661 (88%)	345/409 (84%)	94/122 (77%)

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	74	SER	HB3	2.06	2.49 – 5.20	-6.6

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: