wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2N26 / pdb_00002n26
BMRB ID	:	25587
Title	:	Solution structure of Miz-1 zinc fingers 3 and 4
Authors	:	Bedard, M.; Lavigne, P.
Deposited on	:	2015-04-28

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:

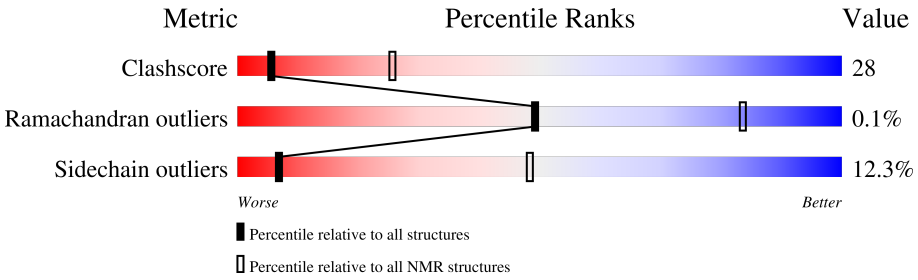
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 87%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	112	21% 22% • • 51%

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 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:59-A:85 (27)	0.37	8
2	A:87-A:110 (24)	0.21	13

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, 2, 3, 4, 6, 7, 8, 9, 10, 11, 12, 14, 15, 16, 17, 18, 19, 20
2	5, 13

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 880 atoms, of which 437 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Zinc finger and BTB domain-containing protein 17.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	55	878	271	437	87	79	4	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q13105

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

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: Zinc finger and BTB domain-containing protein 17

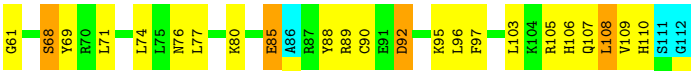
Chain A:

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

The representative model is number 8. Colouring as in section 4.1 above.

• Molecule 1: Zinc finger and BTB domain-containing protein 17

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 300 calculated structures, 20 were deposited, based on the following criterion: *Lowest energy and restraint violations*.

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

Software name	Classification	Version
ARIA	structure calculation	2.2
ARIA	refinement	2.2
CNS	structure calculation	1.21
CNS	refinement	1.21

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	1018
Number of shifts mapped to atoms	647
Number of unparsed shifts	0
Number of shifts with mapping errors	371
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

6 Model quality

6.1 Standard geometry

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	416	411	411	23±3
All	All	8360	8220	8220	457

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 28.

5 of 91 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:LYS:HG3	1:A:85:GLU:HA	0.95	1.36	20	18
1:A:80:LYS:HG2	1:A:85:GLU:HA	0.90	1.42	18	1
1:A:85:GLU:HG3	1:A:87:ARG:HE	0.88	1.26	12	2
1:A:61:GLY:HA2	1:A:68:SER:HA	0.87	1.45	14	20
1:A:93:CYS:SG	1:A:95:LYS:HG3	0.83	2.14	16	13

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	51/112 (46%)	49±0 (96±1%)	2±0 (4±1%)	0±0 (0±0%)	49 83
All	All	1020/2240 (46%)	981 (96%)	38 (4%)	1 (0%)	49 83

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	91	GLU	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	46/98 (47%)	40±1 (88±3%)	6±1 (12±3%)	7 48
All	All	920/1960 (47%)	807 (88%)	113 (12%)	7 48

5 of 17 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	68	SER	20
1	A	108	LEU	20
1	A	64	GLU	17
1	A	76	ASN	16
1	A	71	LEU	9

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 oligosaccharides in this entry.

6.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping

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

Total number of shifts	1018
Number of shifts mapped to atoms	647
Number of unparsed shifts	0
Number of shifts with mapping errors	371
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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 371) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	ILE	C	174.793	.	1
1	A	3	ILE	CA	60.139	0.127	1
1	A	3	ILE	CB	39.322	.	1
1	A	4	HIS	H	8.489	0.005	1
1	A	4	HIS	HA	4.288	.	1
1	A	4	HIS	C	173.614	.	1
1	A	4	HIS	CA	54.233	.	1
1	A	4	HIS	CB	30.216	0.027	1
1	A	4	HIS	N	125.506	0.191	1
1	A	5	LYS	H	8.472	0.004	1
1	A	5	LYS	HA	4.848	.	1
1	A	5	LYS	C	175.057	.	1
1	A	5	LYS	CA	54.572	.	1
1	A	5	LYS	CB	35.314	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	LYS	N	124.514	0.074	1
1	A	6	CYS	H	9.165	0.007	1
1	A	6	CYS	HA	4.462	.	1
1	A	6	CYS	C	177.449	.	1
1	A	6	CYS	CA	59.537	.	1
1	A	6	CYS	CB	29.642	0.007	1
1	A	6	CYS	N	128.563	0.044	1
1	A	7	GLU	H	9.7	0.005	1
1	A	7	GLU	HA	3.973	.	1
1	A	7	GLU	C	176.609	.	1
1	A	7	GLU	CA	58.94	.	1
1	A	7	GLU	CB	29.785	.	1
1	A	7	GLU	N	132.438	0.018	1
1	A	8	ASP	H	8.348	0.015	1
1	A	8	ASP	HA	4.367	.	1
1	A	8	ASP	C	176.809	.	1
1	A	8	ASP	CA	56.93	.	1
1	A	8	ASP	CB	41.101	0.007	1
1	A	8	ASP	N	119.728	0.01	1
1	A	9	CYS	H	7.905	0.006	1
1	A	9	CYS	HA	5.021	.	1
1	A	9	CYS	C	176.131	.	1
1	A	9	CYS	CA	58.495	.	1
1	A	9	CYS	CB	32.163	0.03	1
1	A	9	CYS	N	115.054	0.047	1
1	A	10	GLY	H	8.072	0.005	1
1	A	10	GLY	HA2	3.639	.	2
1	A	10	GLY	HA3	4.116	.	2
1	A	10	GLY	CA	46.184	0.032	1
1	A	10	GLY	N	113.426	0.055	1
1	A	18	ASN	CA	55.408	.	1
1	A	18	ASN	CB	37.195	0.012	1
1	A	19	PHE	H	7.912	0.027	1
1	A	19	PHE	C	175.66	.	1
1	A	19	PHE	CA	60.486	.	1
1	A	19	PHE	CB	39.212	.	1
1	A	19	PHE	N	122.914	0.161	1
1	A	20	LYS	H	8.249	0.007	1
1	A	20	LYS	C	180.33	.	1
1	A	20	LYS	CA	59.281	.	1
1	A	20	LYS	CB	31.55	0.1	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	20	LYS	CD	28.627	.	1
1	A	20	LYS	CG	26.01	.	1
1	A	20	LYS	N	117.574	0.054	1
1	A	21	ARG	H	7.438	0.007	1
1	A	21	ARG	HA	3.742	.	1
1	A	21	ARG	C	178.038	.	1
1	A	21	ARG	CA	58.98	.	1
1	A	21	ARG	CB	30.474	.	1
1	A	21	ARG	N	117.022	0.051	1
1	A	22	HIS	H	7.546	0.005	1
1	A	22	HIS	C	176.764	.	1
1	A	22	HIS	CA	59.445	.	1
1	A	22	HIS	CB	28.45	0.01	1
1	A	22	HIS	N	118.837	0.047	1
1	A	23	ILE	H	7.605	0.004	1
1	A	23	ILE	C	177.744	.	1
1	A	23	ILE	CA	64.98	.	1
1	A	23	ILE	CB	36.77	.	1
1	A	23	ILE	N	111.694	0.039	1
1	A	24	ARG	H	6.697	0.007	1
1	A	24	ARG	C	178.454	.	1
1	A	24	ARG	CA	57.78	.	1
1	A	24	ARG	CB	29.707	.	1
1	A	24	ARG	N	118.44	0.029	1
1	A	25	ILE	H	7.653	0.005	1
1	A	25	ILE	HA	3.724	.	1
1	A	25	ILE	C	177.463	.	1
1	A	25	ILE	CA	63.271	.	1
1	A	25	ILE	CB	37.339	.	1
1	A	25	ILE	N	117.012	0.039	1
1	A	26	HIS	H	6.914	0.003	1
1	A	26	HIS	HA	4.644	.	1
1	A	26	HIS	C	175.839	.	1
1	A	26	HIS	CA	55.499	.	1
1	A	26	HIS	CB	28.458	.	1
1	A	26	HIS	N	117.035	0.077	1
1	A	27	THR	H	7.578	0.005	1
1	A	27	THR	HA	4.109	0.004	1
1	A	27	THR	HB	4.117	0.003	1
1	A	27	THR	HG21	1.058	0.003	1
1	A	27	THR	HG22	1.058	0.003	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	27	THR	HG23	1.058	0.003	1
1	A	27	THR	C	175.349	.	1
1	A	27	THR	CA	62.461	0.018	1
1	A	27	THR	CB	69.607	0.033	1
1	A	27	THR	CG2	21.598	.	1
1	A	27	THR	N	111.784	0.029	1
1	A	28	GLY	H	8.017	0.003	1
1	A	28	GLY	HA2	3.786	0.022	1
1	A	28	GLY	HA3	3.786	0.022	1
1	A	28	GLY	C	173.981	.	1
1	A	28	GLY	CA	45.298	0.056	1
1	A	28	GLY	N	110.039	0.015	1
1	A	29	GLU	H	7.842	0.003	1
1	A	29	GLU	HA	4.012	0.005	1
1	A	29	GLU	HB2	1.801	0.006	2
1	A	29	GLU	HB3	1.832	0.005	2
1	A	29	GLU	HG2	2.104	0.003	2
1	A	29	GLU	HG3	2.045	0.012	2
1	A	29	GLU	C	176.284	.	1
1	A	29	GLU	CA	56.712	0.043	1
1	A	29	GLU	CB	30.371	0.005	1
1	A	29	GLU	CG	36.103	0.013	1
1	A	29	GLU	N	119.56	0.021	1
1	A	30	LYS	H	8.045	0.003	1
1	A	30	LYS	HA	4.322	0.003	1
1	A	30	LYS	HB2	1.431	0.008	1
1	A	30	LYS	HB3	1.431	0.008	1
1	A	30	LYS	HE2	2.748	0.0	1
1	A	30	LYS	HE3	2.748	0.0	1
1	A	30	LYS	CA	53.508	0.053	1
1	A	30	LYS	CB	33.216	0.029	1
1	A	30	LYS	N	121.107	0.02	1
1	A	31	PRO	C	176.006	.	1
1	A	31	PRO	CA	63.355	0.02	1
1	A	31	PRO	CB	31.929	0.023	1
1	A	31	PRO	CG	26.64	.	1
1	A	32	PHE	H	7.675	0.006	1
1	A	32	PHE	HA	4.64	0.009	1
1	A	32	PHE	HB2	2.593	0.011	2
1	A	32	PHE	HB3	2.837	0.005	2
1	A	32	PHE	C	174.591	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	32	PHE	CA	57.23	.	1
1	A	32	PHE	CB	38.877	0.113	1
1	A	32	PHE	N	118.004	0.021	1
1	A	33	SER	H	8.495	0.006	1
1	A	33	SER	HA	5.236	0.005	1
1	A	33	SER	HB2	3.492	0.005	1
1	A	33	SER	HB3	3.491	0.005	1
1	A	33	SER	C	173.751	.	1
1	A	33	SER	CA	56.878	0.07	1
1	A	33	SER	CB	65.16	0.02	1
1	A	33	SER	N	118.145	0.163	1
1	A	34	CYS	H	8.948	0.005	1
1	A	34	CYS	HA	4.291	0.007	1
1	A	34	CYS	HB2	3.307	0.003	2
1	A	34	CYS	HB3	2.991	0.006	2
1	A	34	CYS	C	177.572	.	1
1	A	34	CYS	CA	59.287	0.0	1
1	A	34	CYS	CB	30.579	0.074	1
1	A	34	CYS	N	127.056	0.043	1
1	A	35	ARG	H	9.454	0.013	1
1	A	35	ARG	HA	4.029	0.008	1
1	A	35	ARG	HG2	1.621	0.005	1
1	A	35	ARG	HG3	1.621	0.005	1
1	A	35	ARG	C	176.312	.	1
1	A	35	ARG	CA	58.591	0.002	1
1	A	35	ARG	CB	30.167	0.002	1
1	A	35	ARG	CD	43.193	.	1
1	A	35	ARG	CG	27.11	0.003	1
1	A	35	ARG	N	130.957	0.043	1
1	A	36	GLU	H	9.114	0.016	1
1	A	36	GLU	HA	4.26	0.005	1
1	A	36	GLU	HB2	1.077	0.005	2
1	A	36	GLU	HB3	1.262	0.008	2
1	A	36	GLU	HG2	1.649	0.005	2
1	A	36	GLU	HG3	1.684	0.003	2
1	A	36	GLU	C	176.766	.	1
1	A	36	GLU	CA	57.236	0.047	1
1	A	36	GLU	CB	30.349	0.008	1
1	A	36	GLU	CG	35.038	0.038	1
1	A	36	GLU	N	121.239	0.058	1
1	A	37	CYS	H	8.362	0.008	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	37	CYS	HA	5.0	0.007	1
1	A	37	CYS	HB2	2.645	0.006	2
1	A	37	CYS	HB3	3.296	0.005	2
1	A	37	CYS	C	175.531	.	1
1	A	37	CYS	CA	58.396	0.018	1
1	A	37	CYS	CB	31.879	0.078	1
1	A	37	CYS	N	118.587	0.025	1
1	A	38	SER	H	7.8	0.01	1
1	A	38	SER	HA	4.207	0.007	1
1	A	38	SER	HB2	3.884	0.006	2
1	A	38	SER	HB3	4.049	0.004	2
1	A	38	SER	C	173.194	.	1
1	A	38	SER	CA	60.615	0.021	1
1	A	38	SER	CB	62.269	0.017	1
1	A	38	SER	N	113.959	0.023	1
1	A	39	LYS	H	8.179	0.008	1
1	A	39	LYS	HA	3.788	0.005	1
1	A	39	LYS	HB2	1.034	0.003	2
1	A	39	LYS	HB3	1.516	0.004	2
1	A	39	LYS	HG2	1.094	0.0	1
1	A	39	LYS	HG3	1.094	0.0	1
1	A	39	LYS	C	174.047	.	1
1	A	39	LYS	CA	58.688	0.035	1
1	A	39	LYS	CB	33.472	0.064	1
1	A	39	LYS	CD	29.036	.	1
1	A	39	LYS	CG	25.465	0.013	1
1	A	39	LYS	N	125.288	0.009	1
1	A	40	ALA	H	7.743	0.009	1
1	A	40	ALA	HA	4.91	0.011	1
1	A	40	ALA	HB1	1.145	0.007	1
1	A	40	ALA	HB2	1.145	0.007	1
1	A	40	ALA	HB3	1.145	0.007	1
1	A	40	ALA	C	176.589	.	1
1	A	40	ALA	CA	51.107	0.024	1
1	A	40	ALA	CB	21.618	0.018	1
1	A	40	ALA	N	126.361	0.047	1
1	A	41	PHE	H	8.776	0.005	1
1	A	41	PHE	HA	4.58	0.008	1
1	A	41	PHE	HB2	2.617	0.012	2
1	A	41	PHE	HB3	2.66	0.009	2
1	A	41	PHE	HD1	7.178	0.007	3

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	41	PHE	HD2	7.178	0.007	3
1	A	41	PHE	HE1	6.81	0.002	3
1	A	41	PHE	HE2	6.81	0.002	3
1	A	41	PHE	C	175.13	.	1
1	A	41	PHE	CA	57.185	.	1
1	A	41	PHE	CB	44.105	0.045	1
1	A	41	PHE	CD1	135.295	.	3
1	A	41	PHE	CD2	135.295	.	3
1	A	41	PHE	CE1	133.42	.	3
1	A	41	PHE	CE2	133.42	.	3
1	A	41	PHE	N	116.898	0.031	1
1	A	42	SER	H	9.025	0.006	1
1	A	42	SER	C	173.184	.	1
1	A	42	SER	CA	59.695	0.037	1
1	A	42	SER	CB	63.663	.	1
1	A	42	SER	N	114.712	0.042	1
1	A	43	ASP	H	7.454	0.006	1
1	A	43	ASP	HA	4.983	0.007	1
1	A	43	ASP	HB2	2.609	0.003	2
1	A	43	ASP	HB3	2.657	0.005	2
1	A	43	ASP	CA	50.72	0.045	1
1	A	43	ASP	CB	43.58	0.034	1
1	A	43	ASP	N	120.332	0.018	1
1	A	44	PRO	HA	3.378	0.004	1
1	A	44	PRO	CA	64.304	0.201	1
1	A	44	PRO	CB	30.672	.	1
1	A	45	ALA	H	7.858	0.014	1
1	A	45	ALA	HA	3.876	0.007	1
1	A	45	ALA	HB1	1.247	0.005	1
1	A	45	ALA	HB2	1.247	0.005	1
1	A	45	ALA	HB3	1.247	0.005	1
1	A	45	ALA	C	180.75	.	1
1	A	45	ALA	CA	54.755	0.006	1
1	A	45	ALA	CB	17.811	0.005	1
1	A	45	ALA	N	122.735	0.16	1
1	A	46	ALA	H	7.709	0.003	1
1	A	46	ALA	HA	3.871	0.009	1
1	A	46	ALA	HB1	1.404	0.004	1
1	A	46	ALA	HB2	1.404	0.004	1
1	A	46	ALA	HB3	1.404	0.004	1
1	A	46	ALA	C	179.895	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	46	ALA	CA	54.091	0.016	1
1	A	46	ALA	CB	18.349	0.015	1
1	A	46	ALA	N	123.103	0.015	1
1	A	47	CYS	H	6.98	0.009	1
1	A	47	CYS	HA	3.894	0.001	1
1	A	47	CYS	HB2	2.187	0.013	2
1	A	47	CYS	HB3	2.837	0.004	2
1	A	47	CYS	C	175.509	.	1
1	A	47	CYS	CA	61.379	.	1
1	A	47	CYS	CB	26.05	0.085	1
1	A	47	CYS	N	118.694	0.03	1
1	A	48	LYS	H	7.729	0.005	1
1	A	48	LYS	HA	3.921	0.007	1
1	A	48	LYS	HB2	1.649	0.002	1
1	A	48	LYS	HB3	1.649	0.002	1
1	A	48	LYS	C	178.908	.	1
1	A	48	LYS	CA	59.013	0.005	1
1	A	48	LYS	CB	32.01	0.008	1
1	A	48	LYS	CD	28.716	.	1
1	A	48	LYS	CG	25.346	.	1
1	A	48	LYS	N	119.076	0.039	1
1	A	49	ALA	H	7.702	0.004	1
1	A	49	ALA	HA	3.866	0.009	1
1	A	49	ALA	HB1	1.216	0.011	1
1	A	49	ALA	HB2	1.216	0.011	1
1	A	49	ALA	HB3	1.216	0.011	1
1	A	49	ALA	C	178.953	.	1
1	A	49	ALA	CA	54.749	0.073	1
1	A	49	ALA	CB	17.65	0.062	1
1	A	49	ALA	N	120.055	0.08	1
1	A	50	HIS	H	7.437	0.006	1
1	A	50	HIS	HA	4.156	0.01	1
1	A	50	HIS	HB2	2.899	0.008	2
1	A	50	HIS	HB3	2.987	0.005	2
1	A	50	HIS	HD2	6.611	0.003	1
1	A	50	HIS	HE1	7.864	.	1
1	A	50	HIS	C	178.647	.	1
1	A	50	HIS	CA	58.993	0.044	1
1	A	50	HIS	CB	28.235	0.049	1
1	A	50	HIS	CD2	129.58	.	1
1	A	50	HIS	N	117.102	0.071	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	51	GLU	H	8.918	0.005	1
1	A	51	GLU	HA	3.834	0.004	1
1	A	51	GLU	HB2	1.96	0.003	2
1	A	51	GLU	HB3	2.27	0.003	2
1	A	51	GLU	HG2	2.862	0.006	2
1	A	51	GLU	HG3	3.044	0.008	2
1	A	51	GLU	C	179.013	.	1
1	A	51	GLU	CA	60.395	0.068	1
1	A	51	GLU	CB	30.138	0.106	1
1	A	51	GLU	CG	38.249	0.032	1
1	A	51	GLU	N	123.39	0.059	1
1	A	52	LYS	H	7.116	0.007	1
1	A	52	LYS	HA	4.006	0.003	1
1	A	52	LYS	HB2	1.758	0.003	1
1	A	52	LYS	HB3	1.758	0.003	1
1	A	52	LYS	HG2	1.41	0.008	2
1	A	52	LYS	HG3	1.511	0.008	2
1	A	52	LYS	C	177.746	.	1
1	A	52	LYS	CA	57.904	0.02	1
1	A	52	LYS	CB	32.23	0.02	1
1	A	52	LYS	CD	28.944	.	1
1	A	52	LYS	CG	25.257	0.022	1
1	A	52	LYS	N	116.027	0.041	1
1	A	53	THR	H	7.596	0.013	1
1	A	53	THR	HA	3.998	0.002	1
1	A	53	THR	HB	3.997	0.001	1
1	A	53	THR	HG21	1.117	0.004	1
1	A	53	THR	HG22	1.117	0.004	1
1	A	53	THR	HG23	1.117	0.004	1
1	A	53	THR	C	175.377	.	1
1	A	53	THR	CA	63.341	0.016	1
1	A	53	THR	CB	69.326	0.059	1
1	A	53	THR	CG2	21.086	0.005	1
1	A	53	THR	N	109.1	0.058	1
1	A	54	HIS	H	6.907	0.01	1
1	A	54	HIS	HA	4.46	0.026	1
1	A	54	HIS	HB2	2.905	0.008	2
1	A	54	HIS	HB3	3.072	0.012	2
1	A	54	HIS	HE1	7.847	0.002	1
1	A	54	HIS	CA	55.915	.	1
1	A	54	HIS	CB	28.412	0.007	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	54	HIS	CE1	141.888	.	1
1	A	54	HIS	N	118.589	0.07	1
1	A	56	PRO	HA	4.278	0.014	1
1	A	56	PRO	HB2	1.681	0.007	2
1	A	56	PRO	HB3	2.109	0.004	2
1	A	56	PRO	HD2	3.56	0.005	2
1	A	56	PRO	HD3	3.637	0.011	2
1	A	56	PRO	HG2	1.802	0.004	2
1	A	56	PRO	HG3	1.85	0.003	2
1	A	56	PRO	C	176.565	.	1
1	A	56	PRO	CA	63.065	0.034	1
1	A	56	PRO	CB	31.93	0.058	1
1	A	56	PRO	CD	50.53	0.012	1
1	A	56	PRO	CG	27.131	0.047	1
1	A	57	LEU	H	7.978	0.004	1
1	A	57	LEU	HA	4.041	0.007	1
1	A	57	LEU	HB2	1.347	0.011	2
1	A	57	LEU	HB3	1.445	0.013	2
1	A	57	LEU	HD11	0.706	0.009	2
1	A	57	LEU	HD12	0.706	0.009	2
1	A	57	LEU	HD13	0.706	0.009	2
1	A	57	LEU	HD21	0.745	0.002	2
1	A	57	LEU	HD22	0.745	0.002	2
1	A	57	LEU	HD23	0.745	0.002	2
1	A	57	LEU	CA	55.503	0.041	1
1	A	57	LEU	CB	42.114	0.037	1
1	A	57	LEU	CD1	23.539	0.027	2
1	A	57	LEU	CD2	24.549	0.008	2
1	A	57	LEU	N	121.286	0.067	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
$^{13}C_{\alpha}$	102	0.09 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	94	0.40 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	91	0.13 ± 0.12	None needed (< 0.5 ppm)
^{15}N	96	0.21 ± 0.45	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

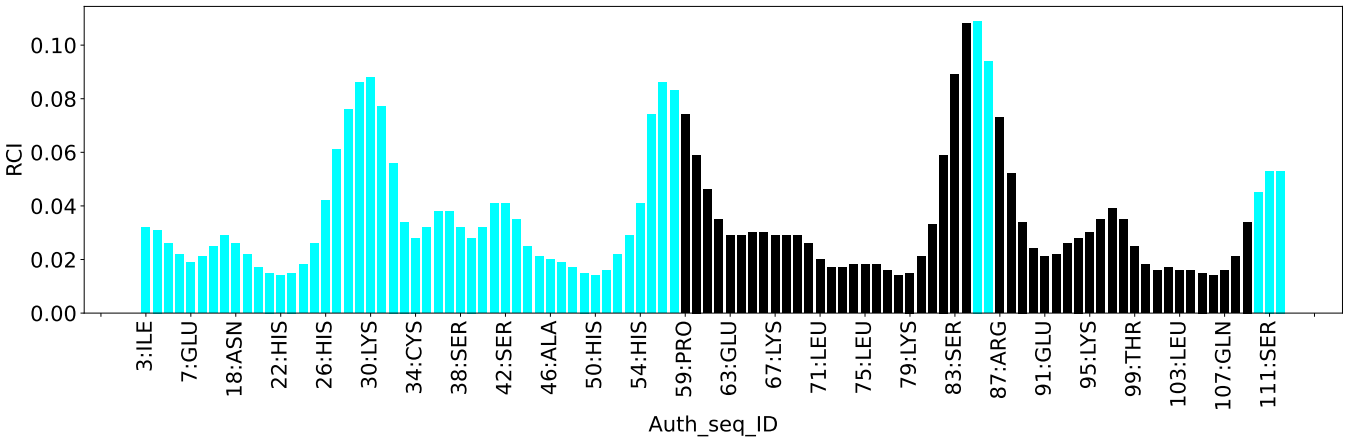
The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 87%, i.e. 622 atoms were assigned a chemical shift out of a possible 717. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	256/258 (99%)	106/106 (100%)	100/102 (98%)	50/50 (100%)
Sidechain	320/394 (81%)	212/252 (84%)	105/119 (88%)	3/23 (13%)
Aromatic	46/65 (71%)	23/33 (70%)	23/28 (82%)	0/4 (0%)
Overall	622/717 (87%)	341/391 (87%)	228/249 (92%)	53/77 (69%)

7.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A: