wwPDB NMR Structure Validation Summary Report

Jun 3, 2023 – 09:00 PM EDT

PDB ID	:	7MC3
BMRB ID	:	50842
Title	:	Solution structure of Miz-1 zinc finger 12
Authors	:	Boisvert, O.; Lavigne, P.
Deposited on	:	2021-04-01

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

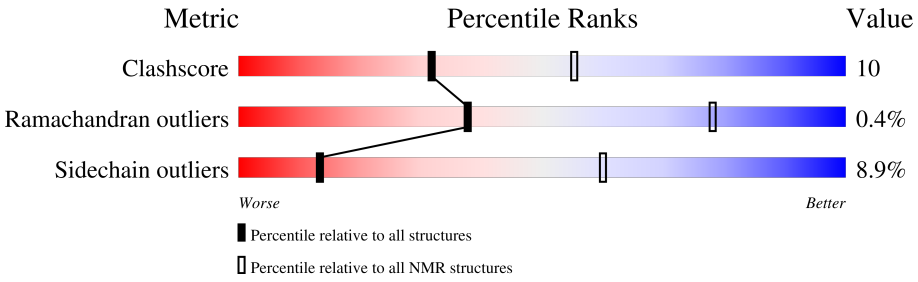
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 78%.

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	85	25% 6% 6% 64%

2 Ensemble composition and analysis

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

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:60-A:85 (26)	0.32	1

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

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

The models can be grouped into 4 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 486 atoms, of which 239 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Isoform 2 of Zinc finger and BTB domain-containing protein 17.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	31	485	149	239	50	45	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q13105
A	32	TYR	HIS	engineered mutation	UNP Q13105

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

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	1	1	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Isoform 2 of 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 1. Colouring as in section 4.1 above.

• Molecule 1: Isoform 2 of 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: *structures with the lowest energy.*

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

Software name	Classification	Version
ARIA	structure calculation	2.3.2
CNS	structure calculation	1.3

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	905
Number of shifts mapped to atoms	326
Number of unparsed shifts	0
Number of shifts with mapping errors	579
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

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	210	203	203	4±2
All	All	4220	4060	4060	79

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 10.

5 of 21 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:LEU:HA	1:A:67:ARG:O	0.69	1.87	8	19
1:A:61:LEU:HB2	1:A:67:ARG:O	0.65	1.91	7	1
1:A:77:SER:O	1:A:81:THR:HG22	0.63	1.94	2	17
1:A:82:VAL:HG13	1:A:83:HIS:CD2	0.53	2.38	2	4
1:A:80:LYS:O	1:A:80:LYS:HD3	0.53	2.02	18	2

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	25/85 (29%)	22±2 (90±7%)	2±2 (10±7%)	0±0 (0±1%)	38 78
All	All	500/1700 (29%)	450 (90%)	48 (10%)	2 (0%)	38 78

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	62	CYS	2

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	23/77 (30%)	21±1 (91±3%)	2±1 (9±3%)	13 60
All	All	460/1540 (30%)	419 (91%)	41 (9%)	13 60

5 of 10 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	71	ARG	20
1	A	61	LEU	9
1	A	84	GLN	3
1	A	81	THR	2
1	A	80	LYS	2

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)

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

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 78% 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	905
Number of shifts mapped to atoms	326
Number of unparsed shifts	0
Number of shifts with mapping errors	579
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 579) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	39	LYS	N	123.915	0.033	1
1	A	32	TYR	HD1	7.242	0.0	1
1	A	32	TYR	HD2	7.242	0.0	1
1	A	47	LEU	HB2	1.893	0.023	2
1	A	39	LYS	HB3	1.401	0.021	2
1	A	38	SER	N	114.203	0.022	1
1	A	39	LYS	HB2	1.419	0.021	2
1	A	47	LEU	HB3	1.893	0.023	2
1	A	14	VAL	CG2	21.596	0.053	2
1	A	4	TYR	HD1	6.958	0.012	1
1	A	4	TYR	HD2	6.958	0.012	1
1	A	13	PHE	HD2	7.019	0.018	1
1	A	13	PHE	HD1	7.019	0.018	1
1	A	13	PHE	HE2	7.027	.	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	13	PHE	HE1	7.027	.	1
1	A	54	HIS	N	117.239	0.072	1
1	A	37	CYS	N	117.691	0.009	1
1	A	45	GLY	N	111.792	0.027	1
1	A	35	SER	N	126.486	0.047	1
1	A	48	SER	N	114.881	0.035	1
1	A	32	TYR	N	118.04	0.153	1
1	A	43	ASN	N	113.174	0.02	1
1	A	53	ILE	N	118.835	0.023	1
1	A	40	ALA	N	123.902	0.019	1
1	A	26	HIS	C	175.52	0.001	1
1	A	41	PHE	HD2	7.229	0.016	1
1	A	41	PHE	HD1	7.229	0.016	1
1	A	32	TYR	HE2	6.919	.	1
1	A	32	TYR	HE1	6.919	.	1
1	A	51	ILE	HG12	1.236	0.008	1
1	A	50	HIS	N	117.984	0.031	1
1	A	47	LEU	N	121.668	0.027	1
1	A	52	ILE	N	117.506	0.073	1
1	A	36	VAL	N	124.529	0.053	1
1	A	41	PHE	N	118.02	0.018	1
1	A	49	LYS	N	118.704	0.063	1
1	A	42	VAL	N	118.084	0.053	1
1	A	51	ILE	N	113.406	0.053	1
1	A	44	VAL	N	121.491	0.038	1
1	A	33	LYS	N	124.426	0.049	1
1	A	34	CYS	N	126.654	0.082	1
1	A	46	ASP	N	121.717	0.034	1
1	A	29	ILE	N	120.52	0.017	1
1	A	29	ILE	CD1	12.69	0.106	1
1	A	29	ILE	CG1	27.031	0.162	1
1	A	29	ILE	CG2	17.479	0.148	1
1	A	29	ILE	HD11	0.747	0.008	1
1	A	29	ILE	HD12	0.747	0.008	1
1	A	29	ILE	HD13	0.747	0.008	1
1	A	28	ASN	C	174.911	0.001	1
1	A	29	ILE	H	7.85	0.017	1
1	A	29	ILE	CA	61.566	0.099	1
1	A	29	ILE	CB	38.06	0.112	1
1	A	27	ASP	N	119.45	0.072	1
1	A	27	ASP	HA	4.547	0.013	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	28	ASN	HD21	7.491	0.013	1
1	A	28	ASN	HD22	6.8	0.011	1
1	A	28	ASN	ND2	112.34	0.04	1
1	A	27	ASP	C	175.913	.	1
1	A	28	ASN	HB2	2.705	0.016	2
1	A	28	ASN	CB	38.78	0.044	1
1	A	28	ASN	HB3	2.705	0.016	2
1	A	28	ASN	CA	53.183	0.106	1
1	A	28	ASN	H	8.186	0.018	1
1	A	28	ASN	HA	4.591	0.027	1
1	A	27	ASP	H	8.1	0.008	1
1	A	25	HIS	H	7.526	0.014	1
1	A	23	ILE	H	7.871	.	1
1	A	22	HIS	H	7.561	0.003	1
1	A	21	ASN	H	7.552	0.014	1
1	A	20	ALA	H	7.929	0.009	1
1	A	10	GLY	H	8.33	0.01	1
1	A	27	ASP	HB2	2.647	0.023	1
1	A	27	ASP	CA	54.68	0.104	1
1	A	27	ASP	CB	40.999	0.021	1
1	A	28	ASN	N	118.563	0.025	1
1	A	29	ILE	HG21	0.806	0.015	1
1	A	29	ILE	HG22	0.806	0.015	1
1	A	29	ILE	HG23	0.806	0.015	1
1	A	29	ILE	HA	4.002	0.012	1
1	A	29	ILE	HB	1.798	0.014	1
1	A	30	ARG	N	124.146	0.049	1
1	A	30	ARG	HA	4.546	0.008	1
1	A	29	ILE	C	175.626	.	1
1	A	30	ARG	HB2	1.542	0.004	1
1	A	30	ARG	CB	30.851	0.05	1
1	A	30	ARG	HD3	2.937	0.005	1
1	A	30	ARG	CA	53.187	0.032	1
1	A	30	ARG	H	8.135	0.004	1
1	A	30	ARG	HG2	1.319	0.024	1
1	A	16	SER	C	177.79	.	1
1	A	17	SER	HB3	4.005	0.014	1
1	A	17	SER	H	8.476	0.004	1
1	A	17	SER	HB2	4.003	0.014	1
1	A	17	SER	CA	60.669	0.016	1
1	A	17	SER	CB	61.435	0.02	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	6	CYS	N	128.483	0.046	1
1	A	6	CYS	HA	4.52	0.005	1
1	A	5	VAL	C	174.458	0.004	1
1	A	6	CYS	HB2	2.772	0.009	2
1	A	8	ARG	HG2	0.641	0.013	1
1	A	8	ARG	HG3	0.641	0.013	1
1	A	11	LYS	N	123.441	0.065	1
1	A	11	LYS	CD	29.448	0.012	1
1	A	11	LYS	HA	3.881	0.007	1
1	A	10	GLY	C	173.685	0.005	1
1	A	11	LYS	CG	26.222	0.009	1
1	A	6	CYS	H	9.043	0.007	1
1	A	13	PHE	H	8.892	0.006	1
1	A	17	SER	N	117.209	0.066	1
1	A	17	SER	HA	4.697	0.021	1
1	A	8	ARG	HB3	1.392	0.007	1
1	A	8	ARG	CB	30.364	0.032	1
1	A	8	ARG	HD3	3.069	0.012	1
1	A	8	ARG	HB2	1.392	0.007	1
1	A	8	ARG	CA	57.841	0.055	1
1	A	8	ARG	HD2	3.069	0.012	1
1	A	8	ARG	H	8.773	0.005	1
1	A	9	CYS	C	176.222	0.003	1
1	A	10	GLY	HA2	3.657	0.012	2
1	A	10	GLY	HA3	4.151	0.01	2
1	A	10	GLY	CA	45.935	0.132	1
1	A	15	GLN	N	114.899	0.019	1
1	A	6	CYS	CA	59.421	0.052	1
1	A	6	CYS	CB	29.665	0.052	1
1	A	6	CYS	HB3	3.312	0.013	2
1	A	8	ARG	CD	42.896	0.01	1
1	A	8	ARG	N	119.93	0.047	1
1	A	8	ARG	HA	4.228	0.012	1
1	A	7	GLU	C	176.592	0.003	1
1	A	8	ARG	CG	26.474	0.053	1
1	A	9	CYS	HA	5.136	0.005	1
1	A	8	ARG	C	177.363	.	1
1	A	9	CYS	HB2	2.828	0.011	2
1	A	9	CYS	H	8.158	0.012	1
1	A	9	CYS	CA	58.479	0.037	1
1	A	9	CYS	CB	32.585	0.059	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	9	CYS	HB3	3.389	0.011	2
1	A	10	GLY	N	113.68	0.038	1
1	A	7	GLU	HG3	2.286	0.022	1
1	A	11	LYS	HB2	1.396	0.012	1
1	A	11	LYS	HB3	1.396	0.012	1
1	A	11	LYS	H	7.995	0.009	1
1	A	11	LYS	CB	33.664	0.059	1
1	A	11	LYS	CA	58.227	0.05	1
1	A	11	LYS	HE2	2.862	0.032	1
1	A	11	LYS	HG2	1.116	0.013	1
1	A	11	LYS	HE3	2.868	0.029	1
1	A	11	LYS	HG3	1.116	0.013	1
1	A	9	CYS	N	115.311	0.052	1
1	A	1	MET	CB	32.836	0.001	1
1	A	1	MET	CG	30.757	0.001	1
1	A	7	GLU	N	132.248	0.08	1
1	A	7	GLU	HA	4.151	0.022	1
1	A	6	CYS	C	177.241	.	1
1	A	7	GLU	HG2	2.286	0.022	1
1	A	7	GLU	HB3	2.063	0.015	1
1	A	7	GLU	CB	29.399	0.046	1
1	A	7	GLU	HB2	2.118	0.014	1
1	A	7	GLU	CA	58.387	0.184	1
1	A	7	GLU	H	9.471	0.01	1
1	A	7	GLU	CG	35.956	0.054	1
1	A	13	PHE	HA	4.758	0.009	1
1	A	15	GLN	HA	4.804	0.006	1
1	A	14	VAL	C	175.977	0.002	1
1	A	15	GLN	H	7.654	0.008	1
1	A	15	GLN	CA	53.789	0.036	1
1	A	15	GLN	CB	31.904	0.013	1
1	A	15	GLN	CG	33.746	0.037	1
1	A	15	GLN	HG3	2.333	0.011	1
1	A	1	MET	CA	55.026	0.017	1
1	A	12	ARG	H	7.681	0.004	1
1	A	12	ARG	HB2	1.484	0.02	1
1	A	12	ARG	CA	54.544	0.053	1
1	A	12	ARG	CB	33.48	0.027	1
1	A	12	ARG	CG	28.332	0.0	1
1	A	24	ARG	N	118.918	0.031	1
1	A	24	ARG	CD	43.457	.	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	24	ARG	H	7.4	0.012	1
1	A	24	ARG	CA	58.426	0.105	1
1	A	24	ARG	CB	30.0	0.063	1
1	A	24	ARG	CG	27.458	.	1
1	A	13	PHE	N	117.956	0.107	1
1	A	22	HIS	CB	28.437	0.062	1
1	A	16	SER	N	121.472	0.05	1
1	A	16	SER	HA	4.693	0.012	1
1	A	15	GLN	C	176.854	.	1
1	A	16	SER	HB3	2.922	0.01	1
1	A	16	SER	CB	61.403	0.232	1
1	A	16	SER	HB2	2.922	0.01	1
1	A	12	ARG	CD	43.476	0.007	1
1	A	12	ARG	N	119.873	0.066	1
1	A	12	ARG	HA	5.091	0.007	1
1	A	11	LYS	C	173.943	0.002	1
1	A	12	ARG	HB3	1.484	0.02	1
1	A	23	ILE	CD1	13.69	0.161	1
1	A	12	ARG	C	175.508	.	1
1	A	13	PHE	CA	56.897	0.074	1
1	A	13	PHE	CB	43.469	0.026	1
1	A	13	PHE	HB2	2.517	0.016	2
1	A	13	PHE	HB3	3.425	0.008	2
1	A	22	HIS	N	119.947	0.032	1
1	A	22	HIS	HA	4.197	0.009	1
1	A	21	ASN	C	176.726	.	1
1	A	22	HIS	HB2	3.211	0.018	1
1	A	22	HIS	CA	59.381	0.08	1
1	A	5	VAL	CA	60.38	0.036	1
1	A	4	TYR	C	174.687	0.003	1
1	A	5	VAL	CG1	21.347	0.157	2
1	A	5	VAL	HG11	0.723	0.015	2
1	A	5	VAL	HG12	0.723	0.015	2
1	A	5	VAL	HG13	0.723	0.015	2
1	A	5	VAL	CB	35.032	0.024	1
1	A	5	VAL	H	8.501	0.01	1
1	A	5	VAL	HB	1.763	0.008	1
1	A	3	PRO	CD	50.637	0.015	1
1	A	3	PRO	CB	32.277	0.024	1
1	A	3	PRO	CA	63.251	0.024	1
1	A	3	PRO	CG	26.806	.	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	20	ALA	CB	17.587	0.06	1
1	A	20	ALA	CA	55.326	0.091	1
1	A	20	ALA	HB3	1.306	0.009	1
1	A	20	ALA	HB1	1.306	0.009	1
1	A	20	ALA	HB2	1.306	0.009	1
1	A	27	ASP	HB3	2.647	0.023	1
1	A	14	VAL	N	118.985	0.051	1
1	A	14	VAL	HA	4.224	0.005	1
1	A	16	SER	CA	61.242	0.024	1
1	A	16	SER	H	8.687	0.005	1
1	A	5	VAL	N	123.393	0.035	1
1	A	5	VAL	HA	4.739	0.015	1
1	A	23	ILE	CA	65.251	0.055	1
1	A	23	ILE	CB	37.903	0.042	1
1	A	23	ILE	HG12	1.772	0.003	1
1	A	23	ILE	CG2	17.496	.	1
1	A	23	ILE	HB	1.769	0.007	1
1	A	23	ILE	HG13	1.772	0.003	1
1	A	20	ALA	N	120.602	0.053	1
1	A	20	ALA	HA	3.944	0.005	1
1	A	19	LEU	C	177.227	.	1
1	A	21	ASN	HD22	6.838	.	1
1	A	21	ASN	CA	56.123	0.199	1
1	A	21	ASN	HD21	6.838	.	1
1	A	21	ASN	HB3	2.734	0.023	2
1	A	4	TYR	N	119.262	0.052	1
1	A	4	TYR	HA	4.56	0.004	1
1	A	3	PRO	C	176.039	.	1
1	A	4	TYR	HB3	2.906	0.019	1
1	A	4	TYR	H	8.066	0.007	1
1	A	4	TYR	CA	57.938	0.039	1
1	A	23	ILE	CG1	29.27	0.06	1
1	A	23	ILE	HA	3.924	0.021	1
1	A	23	ILE	HD11	0.951	0.011	1
1	A	23	ILE	HD12	0.951	0.011	1
1	A	23	ILE	HD13	0.951	0.011	1
1	A	23	ILE	HG21	1.375	0.019	1
1	A	23	ILE	HG22	1.375	0.019	1
1	A	23	ILE	HG23	1.375	0.019	1
1	A	21	ASN	N	115.201	0.086	1
1	A	21	ASN	HA	4.282	0.015	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	20	ALA	C	180.324	.	1
1	A	21	ASN	HB2	2.734	0.023	2
1	A	21	ASN	CB	38.745	0.06	1
1	A	18	GLN	CA	57.597	0.03	1
1	A	18	GLN	H	6.717	0.012	1
1	A	18	GLN	HG3	2.459	0.014	1
1	A	14	VAL	HG11	1.064	0.008	2
1	A	14	VAL	HG12	1.064	0.008	2
1	A	14	VAL	HG13	1.064	0.008	2
1	A	13	PHE	C	175.232	0.0	1
1	A	14	VAL	CG1	21.597	0.058	2
1	A	14	VAL	HG21	1.059	0.012	2
1	A	14	VAL	HG22	1.059	0.012	2
1	A	14	VAL	HG23	1.059	0.012	2
1	A	14	VAL	H	8.681	0.006	1
1	A	14	VAL	CA	64.381	0.021	1
1	A	14	VAL	CB	32.75	0.044	1
1	A	14	VAL	HB	2.26	0.014	1
1	A	19	LEU	H	6.747	0.006	1
1	A	19	LEU	CG	27.211	0.017	1
1	A	19	LEU	HD11	1.063	0.014	2
1	A	19	LEU	HD12	1.063	0.014	2
1	A	19	LEU	HD13	1.063	0.014	2
1	A	18	GLN	N	121.116	0.151	1
1	A	18	GLN	HA	4.013	0.011	1
1	A	18	GLN	HB3	2.027	0.017	1
1	A	17	SER	C	176.855	.	1
1	A	18	GLN	CG	33.967	0.061	1
1	A	18	GLN	CB	28.324	0.066	1
1	A	4	TYR	CB	38.692	0.056	1
1	A	4	TYR	HB2	2.906	0.019	1
1	A	19	LEU	N	121.455	0.032	1
1	A	19	LEU	HA	3.1	0.008	1
1	A	19	LEU	CD2	23.503	1.369	2
1	A	19	LEU	CD1	23.562	1.415	2
1	A	18	GLN	C	178.988	.	1
1	A	19	LEU	CB	40.226	0.07	1
1	A	19	LEU	HB3	1.798	0.009	1
1	A	19	LEU	CA	57.48	0.095	1
1	A	2	LYS	HA	4.689	0.011	1
1	A	2	LYS	HB2	2.128	.	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	LYS	HB3	2.128	.	1
1	A	30	ARG	HB3	1.542	0.004	1
1	A	30	ARG	HD2	2.937	0.005	1
1	A	30	ARG	HG3	1.319	0.024	1
1	A	25	HIS	N	114.897	0.056	1
1	A	25	HIS	HA	4.532	0.012	1
1	A	24	ARG	C	177.471	.	1
1	A	25	HIS	CA	56.138	0.032	1
1	A	25	HIS	HD2	6.917	0.0	1
1	A	25	HIS	CB	28.16	0.137	1
1	A	25	HIS	HB2	3.223	0.017	1
1	A	2	LYS	HG3	1.534	0.013	1
1	A	2	LYS	HG2	1.534	0.013	1
1	A	5	VAL	CG2	20.083	0.034	2
1	A	23	ILE	C	178.347	.	1
1	A	2	LYS	N	125.107	0.038	1
1	A	2	LYS	HE2	3.196	.	1
1	A	1	MET	C	172.026	0.0	1
1	A	2	LYS	CB	32.875	0.016	1
1	A	2	LYS	CA	54.459	0.005	1
1	A	2	LYS	H	8.627	0.009	1
1	A	19	LEU	HG	1.538	0.01	1
1	A	5	VAL	HG21	0.723	0.014	2
1	A	5	VAL	HG22	0.723	0.014	2
1	A	5	VAL	HG23	0.723	0.014	2
1	A	19	LEU	HB2	1.798	0.009	1
1	A	26	HIS	CB	28.992	.	1
1	A	29	ILE	HG13	1.103	0.007	1
1	A	29	ILE	HG12	1.103	0.007	1
1	A	30	ARG	CG	27.403	0.067	1
1	A	26	HIS	CA	57.785	.	1
1	A	24	ARG	HA	4.012	0.003	1
1	A	24	ARG	HB3	1.703	0.006	1
1	A	24	ARG	HB2	1.703	0.006	1
1	A	51	ILE	CB	38.464	0.117	1
1	A	25	HIS	HB3	2.908	0.012	1
1	A	15	GLN	HB3	1.688	0.015	1
1	A	15	GLN	HG2	2.342	0.023	1
1	A	18	GLN	HG2	2.459	0.014	1
1	A	18	GLN	HB2	2.027	0.017	1
1	A	22	HIS	HB3	2.833	0.003	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	15	GLN	HB2	2.233	0.011	1
1	A	19	LEU	HD21	0.962	0.025	2
1	A	19	LEU	HD22	0.962	0.025	2
1	A	19	LEU	HD23	0.962	0.025	2
1	A	44	VAL	HB	1.386	0.015	1
1	A	39	LYS	CD	29.411	0.005	1
1	A	39	LYS	HA	3.884	0.003	1
1	A	39	LYS	C	173.746	0.0	1
1	A	39	LYS	CG	25.956	0.0	1
1	A	39	LYS	CB	33.479	0.023	1
1	A	39	LYS	CA	58.467	0.057	1
1	A	39	LYS	H	8.027	0.006	1
1	A	39	LYS	HG2	1.147	0.019	1
1	A	39	LYS	HG3	1.142	0.014	1
1	A	39	LYS	CE	42.196	0.028	1
1	A	50	HIS	H	7.316	0.005	1
1	A	44	VAL	CG1	21.628	0.672	1
1	A	44	VAL	HA	3.096	0.011	1
1	A	44	VAL	HG12	0.629	0.009	1
1	A	44	VAL	HG13	0.629	0.009	1
1	A	44	VAL	HG11	0.629	0.009	1
1	A	44	VAL	C	177.291	.	1
1	A	44	VAL	HG21	0.63	0.01	1
1	A	44	VAL	HG22	0.63	0.01	1
1	A	44	VAL	HG23	0.63	0.01	1
1	A	44	VAL	CB	31.308	0.09	1
1	A	44	VAL	CA	64.842	0.076	1
1	A	44	VAL	H	8.225	0.008	1
1	A	44	VAL	CG2	21.628	0.672	1
1	A	54	HIS	CA	55.061	0.113	1
1	A	54	HIS	H	7.325	0.005	1
1	A	54	HIS	HB2	3.24	0.023	1
1	A	54	HIS	HB3	3.24	0.023	1
1	A	50	HIS	HA	4.196	0.01	1
1	A	50	HIS	C	176.848	.	1
1	A	50	HIS	HB3	2.862	0.021	1
1	A	50	HIS	CB	29.074	0.004	1
1	A	50	HIS	HB2	2.849	0.024	1
1	A	50	HIS	CA	58.834	0.081	1
1	A	46	ASP	H	7.91	0.01	1
1	A	35	SER	HA	4.718	0.006	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	35	SER	C	174.355	.	1
1	A	35	SER	HB3	4.223	0.023	1
1	A	35	SER	H	8.896	0.014	1
1	A	35	SER	HB2	4.223	0.023	1
1	A	35	SER	CA	60.724	0.123	1
1	A	35	SER	CB	63.216	0.044	1
1	A	54	HIS	HA	4.795	0.014	1
1	A	54	HIS	C	175.607	.	1
1	A	54	HIS	CB	28.447	0.023	1
1	A	34	CYS	H	9.056	0.005	1
1	A	34	CYS	CA	60.034	0.11	1
1	A	34	CYS	CB	29.739	0.006	1
1	A	34	CYS	HB2	2.794	0.012	2
1	A	34	CYS	HB3	3.304	0.02	2
1	A	46	ASP	HA	4.228	0.01	1
1	A	46	ASP	C	178.851	0.001	1
1	A	46	ASP	HB3	2.724	0.013	1
1	A	46	ASP	CB	40.198	0.046	1
1	A	46	ASP	HB2	2.71	0.014	1
1	A	46	ASP	CA	56.555	0.036	1
1	A	40	ALA	CB	22.405	0.012	1
1	A	40	ALA	HB3	1.152	0.005	1
1	A	40	ALA	HB1	1.152	0.005	1
1	A	40	ALA	HB2	1.152	0.005	1
1	A	48	SER	HA	4.183	0.006	1
1	A	48	SER	C	176.127	.	1
1	A	48	SER	HB3	3.963	0.011	1
1	A	48	SER	CB	62.619	0.102	1
1	A	48	SER	HB2	3.963	0.011	1
1	A	48	SER	CA	61.96	0.044	1
1	A	48	SER	H	8.354	0.002	1
1	A	34	CYS	HA	4.419	0.007	1
1	A	34	CYS	C	177.141	.	1
1	A	36	VAL	CB	32.886	0.041	1
1	A	36	VAL	HB	1.098	0.01	1
1	A	36	VAL	HG11	0.274	0.01	2
1	A	36	VAL	HG12	0.274	0.01	2
1	A	36	VAL	HG13	0.274	0.01	2
1	A	36	VAL	HG21	0.814	0.002	2
1	A	36	VAL	HG22	0.814	0.002	2
1	A	36	VAL	HG23	0.814	0.002	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	31	PRO	CA	63.481	.	1
1	A	31	PRO	CB	32.34	.	1
1	A	31	PRO	C	176.458	.	1
1	A	40	ALA	HA	5.053	0.013	1
1	A	40	ALA	C	176.484	0.002	1
1	A	40	ALA	H	7.723	0.008	1
1	A	40	ALA	CA	50.365	0.038	1
1	A	43	ASN	HB2	2.816	0.009	1
1	A	43	ASN	CA	51.672	0.109	1
1	A	43	ASN	H	7.535	0.007	1
1	A	43	ASN	HD21	6.856	0.015	1
1	A	36	VAL	HA	3.806	0.008	1
1	A	36	VAL	C	176.913	0.003	1
1	A	36	VAL	CG1	20.778	0.353	2
1	A	36	VAL	CG2	20.816	0.334	2
1	A	36	VAL	H	8.944	0.007	1
1	A	36	VAL	CA	64.904	0.013	1
1	A	42	VAL	HB	2.213	0.008	1
1	A	43	ASN	HA	4.941	0.006	1
1	A	43	ASN	C	175.016	0.003	1
1	A	43	ASN	HB3	2.816	0.009	1
1	A	43	ASN	CB	41.201	0.029	1
1	A	43	ASN	HD22	6.856	0.015	1
1	A	33	LYS	HB2	1.563	0.006	1
1	A	33	LYS	CA	54.99	0.093	1
1	A	33	LYS	CB	35.175	0.049	1
1	A	33	LYS	CG	25.015	0.069	1
1	A	33	LYS	HE3	2.858	0.013	1
1	A	33	LYS	HG3	1.176	0.012	1
1	A	33	LYS	CE	41.922	.	1
1	A	33	LYS	HE2	2.858	0.013	1
1	A	38	SER	HA	4.149	0.013	1
1	A	38	SER	C	173.01	0.002	1
1	A	38	SER	CB	62.256	0.028	1
1	A	38	SER	CA	61.277	0.022	1
1	A	38	SER	H	7.856	0.008	1
1	A	32	TYR	HB2	2.734	0.015	1
1	A	32	TYR	CA	57.529	0.055	1
1	A	32	TYR	H	7.726	0.018	1
1	A	33	LYS	CD	29.539	.	1
1	A	33	LYS	HA	4.97	0.011	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	33	LYS	C	175.505	.	1
1	A	33	LYS	HG2	1.177	0.012	1
1	A	33	LYS	HB3	1.563	0.006	1
1	A	33	LYS	H	8.553	0.008	1
1	A	41	PHE	HA	4.674	0.011	1
1	A	41	PHE	C	175.336	.	1
1	A	41	PHE	CB	43.626	0.058	1
1	A	41	PHE	CA	57.563	0.039	1
1	A	41	PHE	H	8.797	0.009	1
1	A	41	PHE	HB2	2.624	0.013	2
1	A	41	PHE	HB3	3.407	0.023	2
1	A	32	TYR	HA	4.562	0.013	1
1	A	32	TYR	C	174.551	.	1
1	A	32	TYR	HB3	2.734	0.015	1
1	A	32	TYR	CB	38.711	0.173	1
1	A	45	GLY	C	176.688	0.002	1
1	A	53	ILE	CD1	14.401	0.036	1
1	A	53	ILE	HB	1.836	0.006	1
1	A	53	ILE	CG2	16.425	0.019	1
1	A	53	ILE	HD11	0.629	0.001	1
1	A	53	ILE	HD12	0.629	0.001	1
1	A	53	ILE	HD13	0.629	0.001	1
1	A	53	ILE	C	177.209	.	1
1	A	53	ILE	HG21	0.499	0.001	1
1	A	53	ILE	HG22	0.499	0.001	1
1	A	53	ILE	HG23	0.499	0.001	1
1	A	53	ILE	H	7.722	0.003	1
1	A	53	ILE	CA	63.205	0.02	1
1	A	53	ILE	CB	37.542	0.027	1
1	A	53	ILE	HG12	0.826	.	1
1	A	47	LEU	HD22	0.946	0.013	1
1	A	47	LEU	HD21	0.946	0.013	1
1	A	47	LEU	HD23	0.946	0.013	1
1	A	47	LEU	C	177.717	.	1
1	A	47	LEU	HG	1.545	0.01	1
1	A	47	LEU	H	6.865	0.008	1
1	A	47	LEU	CA	57.841	0.031	1
1	A	47	LEU	CB	40.44	0.052	1
1	A	47	LEU	CG	27.088	0.178	1
1	A	45	GLY	CA	46.666	0.064	1
1	A	45	GLY	HA2	3.74	0.01	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	45	GLY	HA3	3.74	0.01	1
1	A	45	GLY	H	8.431	0.007	1
1	A	37	CYS	H	8.194	0.008	1
1	A	37	CYS	CA	58.329	0.053	1
1	A	37	CYS	CB	32.166	0.019	1
1	A	37	CYS	HB2	3.429	0.007	2
1	A	37	CYS	HB3	2.728	0.012	2
1	A	47	LEU	CD1	22.872	0.028	1
1	A	47	LEU	HA	3.123	0.015	1
1	A	47	LEU	CD2	26.495	0.063	1
1	A	47	LEU	HD12	0.938	0.015	1
1	A	47	LEU	HD11	0.938	0.015	1
1	A	47	LEU	HD13	0.938	0.015	1
1	A	42	VAL	CA	64.085	0.091	1
1	A	42	VAL	C	175.311	0.0	1
1	A	42	VAL	HG21	1.069	0.014	1
1	A	42	VAL	HG22	1.069	0.014	1
1	A	42	VAL	HG23	1.069	0.014	1
1	A	42	VAL	H	9.203	0.003	1
1	A	42	VAL	HG12	1.069	0.014	1
1	A	42	VAL	HG13	1.069	0.014	1
1	A	42	VAL	HG11	1.069	0.014	1
1	A	42	VAL	CB	32.776	0.067	1
1	A	42	VAL	HA	4.209	0.011	1
1	A	42	VAL	CG1	21.514	0.15	1
1	A	37	CYS	HA	5.11	0.009	1
1	A	37	CYS	C	175.681	0.001	1
1	A	49	LYS	CD	29.281	.	1
1	A	49	LYS	HA	3.998	0.006	1
1	A	49	LYS	C	177.569	0.001	1
1	A	49	LYS	HB3	1.693	0.01	1
1	A	49	LYS	CB	32.779	0.046	1
1	A	49	LYS	HB2	1.693	0.01	1
1	A	49	LYS	CA	58.366	0.094	1
1	A	49	LYS	H	7.314	0.006	1
1	A	49	LYS	CG	25.275	.	1
1	A	49	LYS	CE	42.118	0.02	1
1	A	42	VAL	CG2	21.501	0.145	1
1	A	52	ILE	HD11	0.745	0.006	1
1	A	52	ILE	HD12	0.745	0.006	1
1	A	52	ILE	HD13	0.745	0.006	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	52	ILE	C	178.1	0.002	1
1	A	52	ILE	HG21	0.831	0.004	1
1	A	52	ILE	HG22	0.831	0.004	1
1	A	52	ILE	HG23	0.831	0.004	1
1	A	52	ILE	H	6.659	0.006	1
1	A	52	ILE	CA	62.816	0.067	1
1	A	52	ILE	CB	37.864	0.024	1
1	A	52	ILE	HG12	1.291	0.008	1
1	A	52	ILE	CG2	17.978	0.066	1
1	A	52	ILE	HB	1.856	0.005	1
1	A	52	ILE	HG13	1.291	0.008	1
1	A	51	ILE	HD11	0.943	0.002	1
1	A	51	ILE	HD12	0.943	0.002	1
1	A	51	ILE	HD13	0.943	0.002	1
1	A	51	ILE	C	176.897	.	1
1	A	51	ILE	HG21	1.18	0.009	1
1	A	51	ILE	HG22	1.18	0.009	1
1	A	51	ILE	HG23	1.18	0.009	1
1	A	51	ILE	CA	65.419	0.029	1
1	A	51	ILE	HG13	1.236	0.008	1
1	A	51	ILE	H	8.078	0.006	1
1	A	51	ILE	CG2	18.312	0.124	1
1	A	51	ILE	HB	1.968	0.006	1
1	A	52	ILE	CD1	13.326	0.026	1
1	A	52	ILE	CG1	27.641	0.018	1
1	A	52	ILE	HA	3.88	0.012	1
1	A	53	ILE	HA	3.895	0.008	1
1	A	53	ILE	CG1	26.494	0.032	1
1	A	53	ILE	HG13	1.668	0.022	1
1	A	51	ILE	CD1	14.551	0.07	1
1	A	51	ILE	CG1	28.241	.	1
1	A	51	ILE	HA	3.588	0.02	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
$^{13}C_{\alpha}$	85	-0.38 ± 0.39	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	79	0.28 ± 0.16	None needed (< 0.5 ppm)
$^{13}C'$	79	0.00 ± 0.24	None needed (< 0.5 ppm)

Continued on next page...

Continued from previous page...

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
^{15}N	79	0.20 ± 0.77	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 78%, i.e. 283 atoms were assigned a chemical shift out of a possible 361. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	132/133 (99%)	55/55 (100%)	51/52 (98%)	26/26 (100%)
Sidechain	145/195 (74%)	95/124 (77%)	48/57 (84%)	2/14 (14%)
Aromatic	6/33 (18%)	6/17 (35%)	0/14 (0%)	0/2 (0%)
Overall	283/361 (78%)	156/196 (80%)	99/123 (80%)	28/42 (67%)

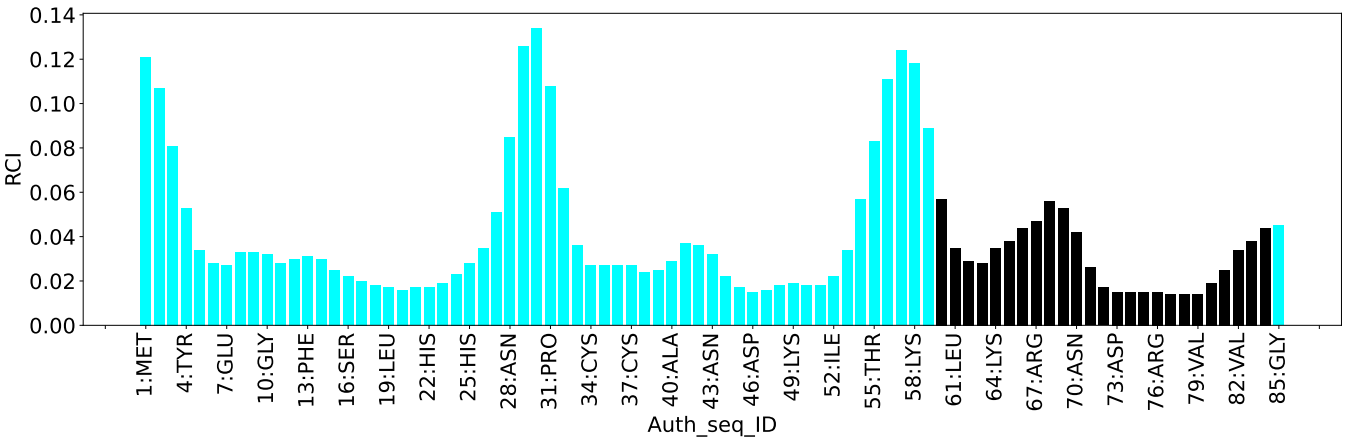
7.1.4 Statistically unusual chemical shifts

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:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	20
Intra-residue (|i-j|=0)	0
Sequential (|i-j|=1)	0
Medium range (|i-j|>1 and |i-j|<5)	0
Long range (|i-j|≥5)	0
Inter-chain	0
Hydrogen bond restraints	20
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.2
Number of long range restraints per residue[1]	0.0

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.There are no distance violations

8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

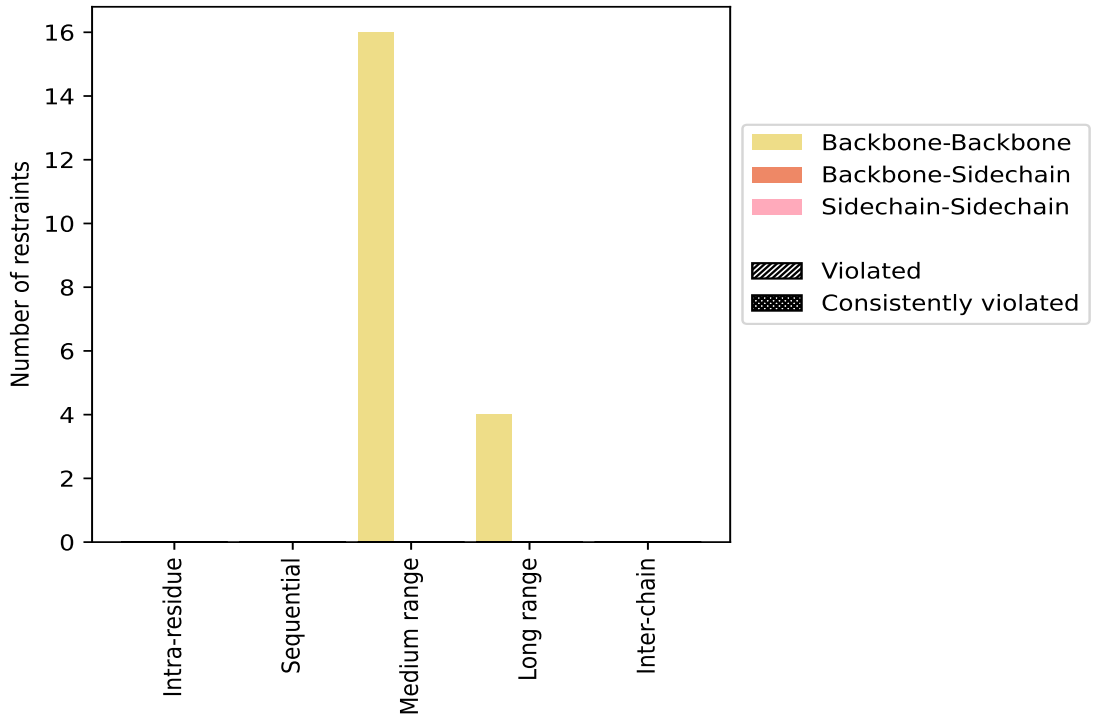
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	20	100.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	20	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	20	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model

No violations found

9.3 Distance violation statistics for the ensemble

No violations found

9.4 Most violated distance restraints in the ensemble

No violations found

9.5 All violated distance restraints

No violations found

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found