wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2M0E
BMRB ID	:	18806
Title	:	Solution Structure of Miz-1 zinc finger 6
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Deposited on	:	2012-10-24

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:

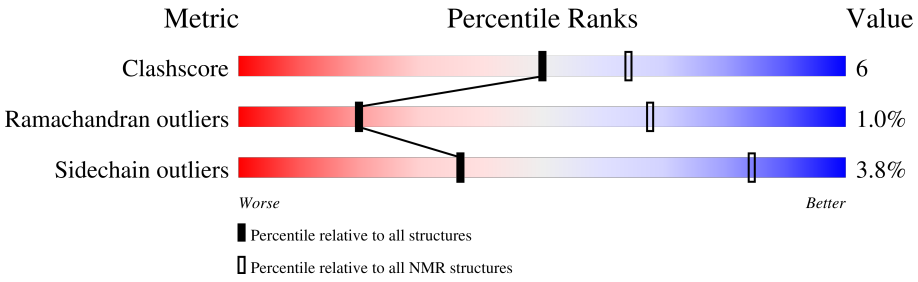
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 76%.

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	112	21% · 74%

2 Ensemble composition and analysis

This entry contains 20 models. Model 18 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:34-A:57 (24)	1.19	18

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 467 atoms, of which 235 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	29	466	145	235	46	38	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q13105

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

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	1	1	1

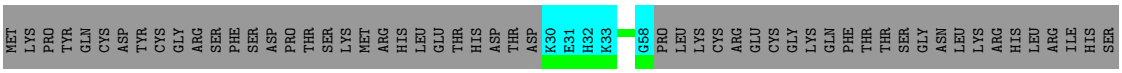
4 Residue-property plots

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: Zinc finger and BTB domain-containing protein 17

Chain A:

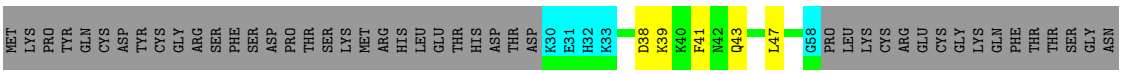


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 18. 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: *structures with the lowest energy.*

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

Software name	Classification	Version
ARIA	refinement	2.2
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	1186
Number of shifts mapped to atoms	270
Number of unparsed shifts	0
Number of shifts with mapping errors	916
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

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	190	192	191	2±2
All	All	3820	3840	3820	46

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 6.

5 of 34 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:PHE:HB2	1:A:46:ASN:HA	0.80	1.52	4	3
1:A:43:GLN:HA	1:A:47:LEU:HB3	0.79	1.54	13	1
1:A:34:CYS:HB3	1:A:37:CYS:HB3	0.76	1.55	2	1
1:A:45:GLY:HA2	1:A:48:LYS:HE2	0.71	1.60	1	1
1:A:34:CYS:HB2	1:A:35:PRO:HD2	0.63	1.71	19	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	24/112 (21%)	22±1 (90±4%)	2±1 (9±3%)	0±1 (1±2%)	20 68
All	All	480/2240 (21%)	432 (90%)	43 (9%)	5 (1%)	20 68

All 2 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	35	PRO	4
1	A	37	CYS	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	21/100 (21%)	20±1 (96±4%)	1±1 (4±4%)	36 84
All	All	420/2000 (21%)	404 (96%)	16 (4%)	36 84

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	54	HIS	3
1	A	37	CYS	2
1	A	38	ASP	2
1	A	39	LYS	2
1	A	34	CYS	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 monosaccharides in this entry.

6.6 Ligand geometry

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

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 76% for the well-defined parts and 67% 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	1186
Number of shifts mapped to atoms	270
Number of unparsed shifts	0
Number of shifts with mapping errors	916
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 916) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	103	LEU	H	6.789	0.009	1
1	A	103	LEU	N	118.329	0.033	1
1	A	103	LEU	CA	57.588	0.064	1
1	A	103	LEU	CB	40.519	0.066	1
1	A	102	ALA	H	8.019	0.005	1
1	A	102	ALA	N	125.555	0.035	1
1	A	102	ALA	CA	54.496	0.046	1
1	A	102	ALA	CB	18.812	0.071	1
1	A	101	GLY	H	8.262	0.01	1
1	A	101	GLY	N	110.226	0.057	1
1	A	101	GLY	CA	46.678	0.054	1
1	A	100	PRO	CA	64.03	0.075	1
1	A	100	PRO	CB	31.142	0.071	1
1	A	99	ASP	H	7.323	0.006	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	99	ASP	N	114.064	0.051	1
1	A	99	ASP	CA	51.162	0.064	1
1	A	99	ASP	CB	42.663	0.035	1
1	A	98	ALA	H	9.019	0.01	1
1	A	98	ALA	N	121.599	0.032	1
1	A	98	ALA	CA	53.297	0.015	1
1	A	98	ALA	CB	19.97	0.057	1
1	A	97	PHE	H	8.875	0.008	1
1	A	97	PHE	N	118.706	0.052	1
1	A	97	PHE	CA	57.285	0.011	1
1	A	97	PHE	CB	43.463	0.069	1
1	A	74	ASN	H	7.74	0.006	1
1	A	74	ASN	N	120.577	0.015	1
1	A	74	ASN	CA	55.21	0.021	1
1	A	74	ASN	CB	37.623	0.079	1
1	A	75	LEU	H	7.343	0.009	1
1	A	75	LEU	N	123.304	0.046	1
1	A	75	LEU	CA	57.968	0.078	1
1	A	75	LEU	CB	40.52	0.079	1
1	A	76	LYS	H	8.254	0.01	1
1	A	76	LYS	N	118.414	0.03	1
1	A	76	LYS	CA	60.272	0.053	1
1	A	15	ASP	H	7.443	0.007	1
1	A	15	ASP	N	117.86	0.028	1
1	A	15	ASP	CA	51.697	0.049	1
1	A	15	ASP	CB	42.344	0.075	1
1	A	13	PHE	H	8.392	0.01	1
1	A	13	PHE	N	118.534	0.06	1
1	A	13	PHE	CA	57.369	0.03	1
1	A	13	PHE	CB	43.443	0.065	1
1	A	14	SER	H	9.09	0.003	1
1	A	14	SER	N	114.545	0.046	1
1	A	14	SER	CA	59.545	0.061	1
1	A	14	SER	CB	64.037	0.072	1
1	A	12	SER	H	7.89	0.011	1
1	A	12	SER	N	115.605	0.048	1
1	A	12	SER	CA	57.311	0.033	1
1	A	12	SER	CB	65.516	0.068	1
1	A	11	ARG	H	7.928	0.008	1
1	A	11	ARG	N	122.427	0.035	1
1	A	11	ARG	CA	57.602	0.011	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	10	GLY	H	7.985	0.013	1
1	A	10	GLY	N	111.402	0.04	1
1	A	5	GLN	H	8.544	0.008	1
1	A	5	GLN	N	123.036	0.04	1
1	A	5	GLN	CA	54.558	0.078	1
1	A	5	GLN	CB	31.592	0.062	1
1	A	4	TYR	H	7.959	0.008	1
1	A	4	TYR	N	117.838	0.034	1
1	A	4	TYR	CA	56.77	0.044	1
1	A	4	TYR	CB	38.43	0.058	1
1	A	3	PRO	CB	31.877	0.043	1
1	A	3	PRO	CA	63.415	0.077	1
1	A	76	LYS	CB	31.908	0.072	1
1	A	77	ARG	H	7.452	0.009	1
1	A	77	ARG	N	117.219	0.057	1
1	A	77	ARG	CA	59.234	0.037	1
1	A	77	ARG	CB	30.442	0.07	1
1	A	78	HIS	H	7.306	0.012	1
1	A	78	HIS	CA	59.113	0.075	1
1	A	78	HIS	CB	28.286	0.065	1
1	A	83	SER	H	7.586	0.007	1
1	A	83	SER	N	114.372	0.051	1
1	A	83	SER	CA	59.132	0.053	1
1	A	83	SER	CB	63.674	0.037	1
1	A	84	GLY	H	8.061	0.005	1
1	A	84	GLY	N	110.203	0.018	1
1	A	84	GLY	CA	45.361	0.07	1
1	A	85	GLU	H	7.881	0.01	1
1	A	85	GLU	N	119.951	0.02	1
1	A	85	GLU	CA	56.641	0.071	1
1	A	85	GLU	CB	30.408	0.042	1
1	A	86	LYS	H	8.079	0.009	1
1	A	86	LYS	N	121.528	0.041	1
1	A	86	LYS	CB	33.098	0.008	1
1	A	86	LYS	CA	53.803	0.006	1
1	A	112	GLY	H	7.878	0.009	1
1	A	112	GLY	N	117.415	0.04	1
1	A	111	THR	H	7.528	0.012	1
1	A	111	THR	N	109.948	0.055	1
1	A	111	THR	CA	62.068	0.059	1
1	A	111	THR	CB	69.863	0.068	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	17	THR	H	7.858	0.007	1
1	A	17	THR	N	117.621	0.047	1
1	A	17	THR	CA	66.554	0.065	1
1	A	17	THR	CB	67.664	0.057	1
1	A	16	PRO	CA	64.377	0.038	1
1	A	16	PRO	CB	31.568	0.07	1
1	A	108	ARG	H	6.735	0.008	1
1	A	108	ARG	N	117.784	0.052	1
1	A	108	ARG	CA	57.871	0.067	1
1	A	108	ARG	CB	29.759	0.041	1
1	A	107	VAL	H	8.352	0.008	1
1	A	107	VAL	N	114.907	0.041	1
1	A	107	VAL	CA	66.042	0.036	1
1	A	107	VAL	CB	31.888	0.07	1
1	A	91	ILE	H	8.687	0.007	1
1	A	91	ILE	N	128.33	0.035	1
1	A	91	ILE	CA	62.872	0.064	1
1	A	91	ILE	CB	37.599	0.048	1
1	A	90	CYS	H	8.869	0.009	1
1	A	90	CYS	N	128.789	0.03	1
1	A	90	CYS	CA	59.226	0.065	1
1	A	90	CYS	CB	29.983	0.071	1
1	A	89	VAL	H	8.195	0.007	1
1	A	89	VAL	N	123.957	0.037	1
1	A	89	VAL	CA	60.879	0.054	1
1	A	89	VAL	CB	34.764	0.029	1
1	A	88	TYR	H	7.917	0.006	1
1	A	88	TYR	N	119.446	0.054	1
1	A	88	TYR	CA	57.597	0.042	1
1	A	88	TYR	CB	37.762	0.058	1
1	A	87	PRO	CB	31.922	0.036	1
1	A	87	PRO	CA	63.071	0.068	1
1	A	72	SER	H	9.243	0.007	1
1	A	72	SER	N	119.177	0.031	1
1	A	72	SER	CA	61.112	0.052	1
1	A	72	SER	CB	62.316	0.04	1
1	A	71	THR	H	7.15	0.011	1
1	A	71	THR	N	108.345	0.042	1
1	A	71	THR	CA	58.874	0.024	1
1	A	71	THR	CB	72.806	0.031	1
1	A	106	HIS	H	7.363	0.01	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	106	HIS	CA	59.059	0.077	1
1	A	106	HIS	CB	28.524	0.075	1
1	A	105	ARG	H	7.707	0.005	1
1	A	105	ARG	N	116.516	0.04	1
1	A	105	ARG	CA	58.968	0.054	1
1	A	105	ARG	CB	30.21	0.055	1
1	A	104	GLN	H	7.861	0.009	1
1	A	104	GLN	N	118.337	0.053	1
1	A	104	GLN	CA	58.869	0.057	1
1	A	104	GLN	CB	27.988	0.053	1
1	A	22	HIS	CA	58.912	0.066	1
1	A	22	HIS	CB	27.921	0.078	1
1	A	93	CYS	H	7.958	0.013	1
1	A	93	CYS	N	115.876	0.021	1
1	A	93	CYS	CA	58.432	0.033	1
1	A	93	CYS	CB	32.158	0.072	1
1	A	94	GLN	H	8.178	0.011	1
1	A	94	GLN	N	116.348	0.034	1
1	A	94	GLN	CB	25.429	0.055	1
1	A	94	GLN	CA	58.288	0.073	1
1	A	95	ARG	H	7.856	0.011	1
1	A	95	ARG	N	121.105	0.053	1
1	A	95	ARG	CA	57.979	0.031	1
1	A	95	ARG	CB	31.403	0.038	1
1	A	96	GLN	H	7.833	0.007	1
1	A	96	GLN	N	119.07	0.045	1
1	A	96	GLN	CB	31.188	0.035	1
1	A	96	GLN	CA	54.273	0.056	1
1	A	9	CYS	H	8.105	0.009	1
1	A	9	CYS	N	115.815	0.047	1
1	A	9	CYS	CA	58.31	0.043	1
1	A	9	CYS	CB	32.273	0.036	1
1	A	8	TYR	H	8.935	0.011	1
1	A	8	TYR	N	119.023	0.036	1
1	A	8	TYR	CA	59.546	0.038	1
1	A	8	TYR	CB	38.06	0.079	1
1	A	7	ASP	H	8.738	0.014	1
1	A	7	ASP	N	129.841	0.02	1
1	A	7	ASP	CA	56.35	0.063	1
1	A	7	ASP	CB	40.743	0.079	1
1	A	6	CYS	H	9.125	0.011	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	6	CYS	N	125.821	0.031	1
1	A	6	CYS	CB	30.278	0.048	1
1	A	6	CYS	CA	60.245	0.074	1
1	A	65	CYS	H	8.115	0.008	1
1	A	65	CYS	N	115.424	0.057	1
1	A	65	CYS	CA	58.223	0.037	1
1	A	65	CYS	CB	32.339	0.061	1
1	A	66	GLY	H	7.984	0.011	1
1	A	66	GLY	N	113.249	0.039	1
1	A	66	GLY	CA	46.164	0.06	1
1	A	67	LYS	H	7.7	0.009	1
1	A	67	LYS	N	122.126	0.044	1
1	A	67	LYS	CA	57.937	0.071	1
1	A	67	LYS	CB	33.563	0.059	1
1	A	68	GLN	H	7.911	0.005	1
1	A	68	GLN	N	120.787	0.059	1
1	A	68	GLN	CA	54.55	0.069	1
1	A	18	SER	H	8.654	0.006	1
1	A	18	SER	N	119.883	0.026	1
1	A	18	SER	CA	61.906	0.051	1
1	A	110	HIS	CA	55.29	0.016	1
1	A	110	HIS	CB	28.463	0.032	1
1	A	92	HIS	CA	57.915	0.038	1
1	A	92	HIS	CB	29.583	0.068	1
1	A	82	HIS	CA	55.064	0.047	1
1	A	82	HIS	CB	28.514	0.032	1
1	A	22	HIS	H	7.374	0.008	1
1	A	22	HIS	N	117.794	0.023	1
1	A	78	HIS	N	119.279	0.042	1
1	A	73	GLY	H	8.661	0.007	1
1	A	73	GLY	N	110.453	0.019	1
1	A	70	THR	CA	62.819	0.028	1
1	A	70	THR	CB	69.591	0.076	1
1	A	21	ARG	CB	30.101	0.061	1
1	A	21	ARG	CA	58.807	0.029	1
1	A	26	HIS	H	7.072	0.013	1
1	A	26	HIS	N	118.044	0.05	1
1	A	26	HIS	CB	28.642	0.039	1
1	A	26	HIS	CA	55.261	.	1
1	A	25	THR	CA	63.499	0.059	1
1	A	25	THR	CB	69.177	0.074	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	25	THR	H	7.557	0.01	1
1	A	25	THR	N	108.89	0.04	1
1	A	24	GLU	CA	58.329	0.058	1
1	A	24	GLU	CB	29.417	0.073	1
1	A	110	HIS	H	7.299	0.008	1
1	A	110	HIS	N	117.512	0.029	1
1	A	109	ILE	CB	37.442	0.052	1
1	A	109	ILE	CA	63.016	0.054	1
1	A	109	ILE	H	7.712	0.01	1
1	A	109	ILE	N	116.281	0.024	1
1	A	64	GLU	CA	57.835	0.022	1
1	A	64	GLU	CB	29.173	0.048	1
1	A	64	GLU	N	120.21	0.058	1
1	A	64	GLU	H	8.674	0.007	1
1	A	63	ARG	CA	58.135	0.061	1
1	A	63	ARG	CB	29.869	0.078	1
1	A	63	ARG	H	9.213	0.008	1
1	A	63	ARG	N	131.833	0.032	1
1	A	62	CYS	CA	59.489	0.046	1
1	A	62	CYS	CB	29.664	0.074	1
1	A	62	CYS	H	9.008	0.012	1
1	A	62	CYS	N	127.047	0.06	1
1	A	61	LYS	CA	54.322	0.054	1
1	A	61	LYS	CB	35.449	0.035	1
1	A	61	LYS	H	7.587	0.01	1
1	A	61	LYS	N	120.279	0.057	1
1	A	60	LEU	H	8.314	0.009	1
1	A	60	LEU	N	120.479	0.034	1
1	A	59	PRO	CA	63.48	0.064	1
1	A	59	PRO	CB	31.639	.	1
1	A	70	THR	H	9.023	0.005	1
1	A	70	THR	N	108.936	0.034	1
1	A	69	PHE	CA	57.347	0.051	1
1	A	69	PHE	CB	43.408	0.061	1
1	A	69	PHE	H	8.308	0.01	1
1	A	69	PHE	N	120.205	0.059	1
1	A	82	HIS	H	6.975	0.013	1
1	A	82	HIS	N	117.229	0.046	1
1	A	81	ILE	CB	37.27	0.061	1
1	A	81	ILE	CA	63.01	0.058	1
1	A	81	ILE	H	7.763	0.009	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	81	ILE	N	116.941	0.024	1
1	A	80	ARG	CA	58.327	0.054	1
1	A	80	ARG	CB	29.806	0.043	1
1	A	80	ARG	H	6.954	0.011	1
1	A	80	ARG	N	116.912	0.049	1
1	A	79	LEU	CB	41.703	0.061	1
1	A	79	LEU	CA	57.964	0.034	1
1	A	19	LYS	H	6.76	0.009	1
1	A	19	LYS	N	121.563	0.025	1
1	A	19	LYS	CA	59.487	0.059	1
1	A	19	LYS	CB	31.586	0.011	1
1	A	21	ARG	H	8.066	0.01	1
1	A	21	ARG	N	118.164	0.029	1
1	A	20	MET	CB	31.756	0.074	1
1	A	20	MET	CA	58.719	0.028	1
1	A	111	THR	C	174.74	.	1
1	A	110	HIS	C	175.597	.	1
1	A	109	ILE	C	176.877	.	1
1	A	108	ARG	C	178.341	.	1
1	A	107	VAL	C	176.81	.	1
1	A	106	HIS	C	176.619	.	1
1	A	105	ARG	C	178.351	.	1
1	A	104	GLN	C	178.34	.	1
1	A	103	LEU	C	176.809	.	1
1	A	102	ALA	C	180.54	.	1
1	A	101	GLY	C	175.852	.	1
1	A	100	PRO	C	178.935	.	1
1	A	98	ALA	C	176.342	.	1
1	A	97	PHE	C	174.888	.	1
1	A	96	GLN	C	174.982	.	1
1	A	95	ARG	C	174.113	.	1
1	A	94	GLN	C	174.707	.	1
1	A	93	CYS	C	174.973	.	1
1	A	92	HIS	C	176.698	.	1
1	A	90	CYS	C	177.11	.	1
1	A	89	VAL	C	175.019	.	1
1	A	88	TYR	C	174.419	.	1
1	A	87	PRO	C	176.103	.	1
1	A	85	GLU	C	176.197	.	1
1	A	84	GLY	C	174.031	.	1
1	A	83	SER	C	174.859	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	82	HIS	C	175.365	.	1
1	A	81	ILE	C	177.513	.	1
1	A	79	LEU	C	178.932	.	1
1	A	80	ARG	C	178.644	.	1
1	A	77	ARG	C	178.514	.	1
1	A	76	LYS	C	179.149	.	1
1	A	72	SER	C	177.313	.	1
1	A	71	THR	C	174.614	.	1
1	A	70	THR	C	175.435	.	1
1	A	69	PHE	C	175.241	.	1
1	A	68	GLN	C	174.813	.	1
1	A	67	LYS	C	174.006	.	1
1	A	66	GLY	C	173.337	.	1
1	A	65	CYS	C	176.295	.	1
1	A	64	GLU	C	177.231	.	1
1	A	63	ARG	C	176.307	.	1
1	A	62	CYS	C	177.533	.	1
1	A	61	LYS	C	175.533	.	1
1	A	60	LEU	C	174.836	.	1
1	A	59	PRO	C	176.875	.	1
1	A	75	LEU	C	177.097	.	1
1	A	74	ASN	C	177.974	.	1
1	A	73	GLY	C	176.236	.	1
1	A	25	THR	C	175.17	.	1
1	A	24	GLU	C	178.251	.	1
1	A	21	ARG	C	179.107	.	1
1	A	20	MET	C	178.91	.	1
1	A	18	SER	C	177.038	.	1
1	A	17	THR	C	176.424	.	1
1	A	16	PRO	C	178.801	.	1
1	A	14	SER	C	173.113	.	1
1	A	13	PHE	C	175.33	.	1
1	A	12	SER	C	172.775	.	1
1	A	11	ARG	C	174.22	.	1
1	A	10	GLY	C	173.932	.	1
1	A	9	CYS	C	175.815	.	1
1	A	8	TYR	C	176.44	.	1
1	A	7	ASP	C	175.676	.	1
1	A	6	CYS	C	176.578	.	1
1	A	5	GLN	C	175.122	.	1
1	A	4	TYR	C	174.569	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	PRO	C	176.083	.	1
1	A	24	GLU	H	7.122	0.012	1
1	A	24	GLU	N	116.297	0.04	1
1	A	23	LEU	CA	58.592	0.067	1
1	A	23	LEU	CB	41.658	0.064	1
1	A	23	LEU	C	179.021	.	1
1	A	23	LEU	H	8.385	0.01	1
1	A	23	LEU	N	122.319	0.052	1
1	A	22	HIS	C	178.014	.	1
1	A	20	MET	H	7.831	0.01	1
1	A	20	MET	N	118.908	0.012	1
1	A	19	LYS	C	176.639	.	1
1	A	92	HIS	H	8.526	0.015	1
1	A	92	HIS	N	121.59	0.059	1
1	A	91	ILE	C	175.617	.	1
1	A	111	THR	CG2	21.179	0.058	1
1	A	109	ILE	CG1	26.404	0.037	1
1	A	109	ILE	CG2	16.582	0.078	1
1	A	109	ILE	CD1	14.638	0.053	1
1	A	108	ARG	CG	27.003	0.006	1
1	A	108	ARG	CD	43.062	0.065	1
1	A	105	ARG	CG	28.003	0.008	1
1	A	105	ARG	CD	43.004	0.009	1
1	A	104	GLN	CG	33.706	0.078	1
1	A	103	LEU	CD2	23.359	0.026	2
1	A	103	LEU	CG	26.606	.	1
1	A	107	VAL	CG2	21.848	0.048	2
1	A	100	PRO	CG	26.824	0.024	1
1	A	100	PRO	CD	50.016	0.034	1
1	A	96	GLN	CG	34.06	.	1
1	A	95	ARG	CG	28.398	0.018	1
1	A	95	ARG	CD	43.547	0.078	1
1	A	94	GLN	CG	34.36	0.054	1
1	A	89	VAL	CG2	20.584	0.048	2
1	A	87	PRO	CG	26.478	0.076	1
1	A	87	PRO	CD	49.706	0.016	1
1	A	85	GLU	CG	36.14	0.054	1
1	A	80	ARG	CG	27.104	0.009	1
1	A	80	ARG	CD	43.397	0.007	1
1	A	79	LEU	CG	24.335	0.049	1
1	A	79	LEU	CD2	25.641	0.055	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	79	LEU	CD1	25.641	0.055	1
1	A	77	ARG	CG	27.98	0.018	1
1	A	77	ARG	CD	43.205	0.01	1
1	A	76	LYS	CG	25.9	0.001	1
1	A	76	LYS	CD	29.27	0.048	1
1	A	76	LYS	CE	41.796	0.008	1
1	A	70	THR	CG2	22.256	0.075	1
1	A	68	GLN	CG	34.108	0.045	1
1	A	67	LYS	CG	26.138	.	1
1	A	67	LYS	CD	28.967	0.043	1
1	A	67	LYS	CE	42.133	0.037	1
1	A	64	GLU	CG	35.257	0.051	1
1	A	63	ARG	CG	27.124	0.035	1
1	A	63	ARG	CD	43.293	0.028	1
1	A	61	LYS	CG	25.191	.	1
1	A	61	LYS	CD	29.395	0.01	1
1	A	61	LYS	CE	41.411	0.018	1
1	A	60	LEU	CD2	25.524	0.06	2
1	A	75	LEU	CD1	26.273	0.058	2
1	A	75	LEU	CD2	22.725	0.056	2
1	A	25	THR	CG2	21.666	0.065	1
1	A	24	GLU	CG	36.091	0.055	1
1	A	23	LEU	CD1	24.716	0.047	2
1	A	23	LEU	CD2	25.93	0.044	2
1	A	21	ARG	CG	27.802	0.004	1
1	A	21	ARG	CD	43.078	.	1
1	A	20	MET	CG	31.692	0.036	1
1	A	19	LYS	CG	25.3	0.002	1
1	A	19	LYS	CD	28.802	.	1
1	A	19	LYS	CE	43.094	.	1
1	A	17	THR	CG2	21.805	0.071	1
1	A	16	PRO	CG	26.727	.	1
1	A	16	PRO	CD	49.9	0.0	1
1	A	11	ARG	CG	27.904	0.008	1
1	A	11	ARG	CD	43.278	0.019	1
1	A	5	GLN	CG	33.813	0.038	1
1	A	3	PRO	CG	27.125	.	1
1	A	3	PRO	CD	50.236	.	1
1	A	59	PRO	CG	26.989	0.039	1
1	A	59	PRO	CD	49.803	0.018	1
1	A	91	ILE	CG1	28.529	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	91	ILE	CG2	17.542	0.027	1
1	A	91	ILE	CD1	13.948	.	1
1	A	109	ILE	HG21	0.441	0.015	1
1	A	109	ILE	HG22	0.441	0.015	1
1	A	109	ILE	HG23	0.441	0.015	1
1	A	109	ILE	HD11	0.526	0.013	1
1	A	109	ILE	HD12	0.526	0.013	1
1	A	109	ILE	HD13	0.526	0.013	1
1	A	109	ILE	HG13	0.815	0.015	2
1	A	109	ILE	HG12	0.754	0.015	2
1	A	109	ILE	HB	1.548	0.013	1
1	A	109	ILE	HA	3.813	0.015	1
1	A	20	MET	HE1	1.933	0.014	1
1	A	20	MET	HE2	1.933	0.014	1
1	A	20	MET	HE3	1.933	0.014	1
1	A	20	MET	CE	16.78	0.058	1
1	A	102	ALA	HA	3.817	0.012	1
1	A	102	ALA	HB1	1.465	0.011	1
1	A	102	ALA	HB2	1.465	0.011	1
1	A	102	ALA	HB3	1.465	0.011	1
1	A	98	ALA	HB1	1.454	0.011	1
1	A	98	ALA	HB2	1.454	0.011	1
1	A	98	ALA	HB3	1.454	0.011	1
1	A	98	ALA	HA	4.462	0.014	1
1	A	70	THR	HG21	1.123	0.014	1
1	A	70	THR	HG22	1.123	0.014	1
1	A	70	THR	HG23	1.123	0.014	1
1	A	70	THR	HB	4.284	0.007	1
1	A	70	THR	HA	4.267	0.009	1
1	A	111	THR	HG21	0.991	0.014	1
1	A	111	THR	HG22	0.991	0.014	1
1	A	111	THR	HG23	0.991	0.014	1
1	A	111	THR	HA	4.135	0.015	1
1	A	111	THR	HB	4.176	0.014	1
1	A	25	THR	HA	4.01	0.013	1
1	A	25	THR	HB	3.921	0.014	1
1	A	25	THR	HG21	1.091	0.015	1
1	A	25	THR	HG22	1.091	0.015	1
1	A	25	THR	HG23	1.091	0.015	1
1	A	17	THR	HG21	1.038	0.013	1
1	A	17	THR	HG22	1.038	0.013	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	17	THR	HG23	1.038	0.013	1
1	A	17	THR	HB	4.031	0.009	1
1	A	17	THR	HA	3.759	0.015	1
1	A	84	GLY	HA3	3.816	0.013	1
1	A	84	GLY	HA2	3.816	0.013	1
1	A	100	PRO	HD3	3.617	0.01	2
1	A	100	PRO	HD2	3.025	0.008	2
1	A	100	PRO	HB2	1.712	0.012	2
1	A	100	PRO	HB3	1.641	0.011	2
1	A	100	PRO	HG3	1.811	0.014	2
1	A	100	PRO	HG2	1.556	0.007	2
1	A	1	MET	CE	19.935	0.024	1
1	A	1	MET	HE1	1.616	0.013	1
1	A	1	MET	HE2	1.616	0.013	1
1	A	1	MET	HE3	1.616	0.013	1
1	A	99	ASP	HB3	2.666	0.013	2
1	A	99	ASP	HB2	2.535	0.014	2
1	A	99	ASP	HA	4.742	0.013	1
1	A	75	LEU	HD21	0.704	0.013	2
1	A	75	LEU	HD22	0.704	0.013	2
1	A	75	LEU	HD23	0.704	0.013	2
1	A	75	LEU	HD11	0.793	0.011	2
1	A	75	LEU	HD12	0.793	0.011	2
1	A	75	LEU	HD13	0.793	0.011	2
1	A	75	LEU	HB3	1.841	0.013	2
1	A	75	LEU	HA	2.948	0.013	1
1	A	23	LEU	HA	3.784	0.013	1
1	A	23	LEU	HB3	1.912	0.012	2
1	A	23	LEU	HB2	1.598	0.014	2
1	A	23	LEU	HD11	1.146	0.014	2
1	A	23	LEU	HD12	1.146	0.014	2
1	A	23	LEU	HD13	1.146	0.014	2
1	A	23	LEU	HD21	1.002	0.013	2
1	A	23	LEU	HD22	1.002	0.013	2
1	A	23	LEU	HD23	1.002	0.013	2
1	A	79	LEU	HG	1.083	0.013	1
1	A	79	LEU	HD11	0.84	0.013	1
1	A	79	LEU	HD12	0.84	0.013	1
1	A	79	LEU	HD13	0.84	0.013	1
1	A	79	LEU	HD21	0.84	0.013	1
1	A	79	LEU	HD22	0.84	0.013	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	79	LEU	HD23	0.84	0.013	1
1	A	79	LEU	HB3	1.755	0.011	2
1	A	79	LEU	HB2	1.415	0.014	2
1	A	79	LEU	HA	3.643	0.013	1
1	A	79	LEU	N	116.633	0.031	1
1	A	79	LEU	H	8.084	0.009	1
1	A	78	HIS	C	175.93	.	1
1	A	7	ASP	HA	4.216	0.012	1
1	A	7	ASP	HB3	2.309	0.013	2
1	A	7	ASP	HB2	1.901	0.012	2
1	A	24	GLU	HA	3.992	0.012	1
1	A	24	GLU	HB2	1.983	0.011	1
1	A	24	GLU	HB3	1.983	0.011	1
1	A	24	GLU	HG3	2.4	0.011	2
1	A	24	GLU	HG2	2.2	0.014	2
1	A	104	GLN	HA	3.8	0.011	1
1	A	104	GLN	HG3	2.304	0.009	2
1	A	104	GLN	HG2	2.22	0.015	2
1	A	104	GLN	HB2	1.99	0.014	1
1	A	104	GLN	HB3	1.99	0.014	1
1	A	85	GLU	HB3	1.873	0.012	2
1	A	85	GLU	HB2	1.807	0.012	2
1	A	85	GLU	HG3	2.141	0.009	2
1	A	85	GLU	HG2	2.113	0.014	2
1	A	85	GLU	HA	4.085	0.012	1
1	A	62	CYS	HB3	3.195	0.013	2
1	A	62	CYS	HB2	2.727	0.01	2
1	A	62	CYS	HA	4.349	0.013	1
1	A	90	CYS	HA	4.504	0.013	1
1	A	90	CYS	HB3	3.275	0.01	2
1	A	90	CYS	HB2	2.753	0.012	2
1	A	6	CYS	HA	4.277	0.014	1
1	A	6	CYS	HB3	2.863	0.013	2
1	A	6	CYS	HB2	3.368	0.012	2
1	A	95	ARG	HA	3.927	0.012	1
1	A	11	ARG	HA	3.928	0.014	1
1	A	11	ARG	HD3	2.949	0.011	2
1	A	11	ARG	HD2	2.752	0.014	2
1	A	95	ARG	HD2	2.758	0.009	2
1	A	95	ARG	HD3	2.976	0.008	2
1	A	95	ARG	HB2	1.354	0.012	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	95	ARG	HB3	1.201	0.015	2
1	A	11	ARG	HB3	1.346	0.013	2
1	A	11	ARG	CB	31.248	0.044	1
1	A	11	ARG	HB2	1.197	0.015	2
1	A	11	ARG	HG3	1.704	0.011	2
1	A	11	ARG	HG2	1.668	0.015	2
1	A	95	ARG	HG2	1.705	0.011	2
1	A	95	ARG	HG3	1.671	0.015	2
1	A	107	VAL	CG1	22.376	0.024	2
1	A	107	VAL	HG21	1.191	0.014	2
1	A	107	VAL	HG22	1.191	0.014	2
1	A	107	VAL	HG23	1.191	0.014	2
1	A	107	VAL	HG11	1.257	0.013	2
1	A	107	VAL	HG12	1.257	0.013	2
1	A	107	VAL	HG13	1.257	0.013	2
1	A	107	VAL	HB	2.207	0.014	1
1	A	107	VAL	HA	3.473	0.012	1
1	A	89	VAL	CG1	21.513	0.065	2
1	A	89	VAL	HG21	0.599	0.013	2
1	A	89	VAL	HG22	0.599	0.013	2
1	A	89	VAL	HG23	0.599	0.013	2
1	A	89	VAL	HG11	0.649	0.011	2
1	A	89	VAL	HG12	0.649	0.011	2
1	A	89	VAL	HG13	0.649	0.011	2
1	A	89	VAL	HB	1.702	0.013	1
1	A	89	VAL	HA	4.578	0.011	1
1	A	106	HIS	HA	4.103	0.014	1
1	A	60	LEU	HB3	1.618	0.015	2
1	A	60	LEU	CB	41.692	0.037	1
1	A	60	LEU	HB2	1.426	0.01	2
1	A	60	LEU	CA	54.188	0.06	1
1	A	60	LEU	HA	4.313	0.011	1
1	A	60	LEU	CG	26.901	0.003	1
1	A	60	LEU	HG	1.424	0.013	1
1	A	60	LEU	HD21	0.61	0.012	1
1	A	60	LEU	HD22	0.61	0.012	1
1	A	60	LEU	HD23	0.61	0.012	1
1	A	60	LEU	CD1	23.005	0.045	2
1	A	60	LEU	HD11	0.585	0.015	1
1	A	60	LEU	HD12	0.585	0.015	1
1	A	60	LEU	HD13	0.585	0.015	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	94	GLN	HG2	2.099	0.015	1
1	A	94	GLN	HG3	2.099	0.015	1
1	A	94	GLN	HB3	2.186	0.007	2
1	A	94	GLN	HB2	2.306	0.011	2
1	A	94	GLN	HA	3.876	0.012	1
1	A	68	GLN	CB	31.199	0.003	1
1	A	63	ARG	HD2	3.085	0.013	1
1	A	63	ARG	HD3	3.085	0.013	1
1	A	63	ARG	HA	3.996	0.015	1
1	A	63	ARG	HB2	1.789	0.013	1
1	A	63	ARG	HB3	1.789	0.013	1
1	A	63	ARG	HG3	1.586	0.013	1
1	A	63	ARG	HG2	1.586	0.013	1
1	A	20	MET	HG3	2.049	0.013	1
1	A	20	MET	HG2	2.049	0.013	1
1	A	20	MET	HB3	2.496	0.014	2
1	A	20	MET	HB2	2.527	0.014	2
1	A	20	MET	HA	3.927	0.012	1
1	A	71	THR	HA	4.732	0.002	1
1	A	71	THR	HB	4.444	0.014	1
1	A	71	THR	HG21	1.107	0.011	1
1	A	71	THR	HG22	1.107	0.011	1
1	A	71	THR	HG23	1.107	0.011	1
1	A	72	SER	HB3	3.807	0.015	1
1	A	72	SER	HB2	3.807	0.015	1
1	A	72	SER	HA	3.9	0.013	1
1	A	3	PRO	HA	4.147	0.006	1
1	A	3	PRO	HD3	3.614	0.01	2
1	A	3	PRO	HD2	3.477	0.012	2
1	A	3	PRO	HB3	1.923	0.01	2
1	A	3	PRO	HB2	1.312	0.009	2
1	A	3	PRO	HG2	1.693	0.01	1
1	A	15	ASP	HB3	2.724	0.012	2
1	A	15	ASP	HB2	2.561	0.015	2
1	A	15	ASP	HA	4.704	0.009	1
1	A	8	TYR	HB3	2.384	0.014	2
1	A	8	TYR	HA	4.24	0.007	1
1	A	66	GLY	HA2	3.63	0.013	2
1	A	66	GLY	HA3	4.08	0.014	2
1	A	67	LYS	HA	3.824	0.009	1
1	A	67	LYS	HE3	2.836	0.011	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	67	LYS	HE2	2.798	0.009	2
1	A	67	LYS	HB3	1.317	0.007	2
1	A	67	LYS	HB2	1.082	0.015	2
1	A	67	LYS	HD2	1.335	0.009	1
1	A	67	LYS	HD3	1.335	0.009	1
1	A	5	GLN	HA	4.877	0.013	1
1	A	5	GLN	HB2	1.708	0.008	1
1	A	5	GLN	HB3	1.708	0.008	1
1	A	5	GLN	HG3	2.02	0.015	1
1	A	5	GLN	HG2	2.02	0.015	1
1	A	10	GLY	HA3	3.753	0.011	2
1	A	10	GLY	HA2	4.05	0.01	2
1	A	10	GLY	CA	46.039	0.043	1
1	A	101	GLY	HA2	3.63	0.011	1
1	A	101	GLY	HA3	3.63	0.011	1
1	A	68	GLN	HE21	6.72	0.01	1
1	A	68	GLN	NE2	111.914	0.054	1
1	A	68	GLN	HE22	7.445	0.009	1
1	A	94	GLN	HE22	6.368	0.004	1
1	A	104	GLN	HE22	7.476	0.011	1
1	A	104	GLN	NE2	111.002	0.052	1
1	A	94	GLN	HE21	7.129	0.01	1
1	A	94	GLN	NE2	112.157	0.053	1
1	A	104	GLN	HE21	6.657	0.015	1
1	A	74	ASN	HA	4.397	0.012	1
1	A	74	ASN	HB3	2.821	0.013	1
1	A	74	ASN	HB2	2.821	0.013	1
1	A	4	TYR	HB3	2.825	0.012	2
1	A	4	TYR	HB2	2.651	0.013	2
1	A	4	TYR	HA	4.46	0.013	1
1	A	13	PHE	HB3	3.293	0.012	2
1	A	13	PHE	HB2	2.574	0.014	2
1	A	13	PHE	HA	4.591	0.009	1
1	A	112	GLY	HA3	3.548	0.014	2
1	A	112	GLY	CA	46.168	0.065	1
1	A	112	GLY	HA2	3.751	0.011	2
1	A	73	GLY	CA	46.952	0.067	1
1	A	73	GLY	HA2	3.804	0.014	1
1	A	73	GLY	HA3	3.804	0.014	1
1	A	65	CYS	HA	5.028	0.01	1
1	A	93	CYS	HA	5.023	0.007	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	93	CYS	HB3	2.723	0.014	2
1	A	93	CYS	HB2	3.312	0.015	2
1	A	92	HIS	HA	4.204	0.013	1
1	A	65	CYS	HB3	3.309	0.012	2
1	A	65	CYS	HB2	2.723	0.011	2
1	A	9	CYS	HA	5.038	0.011	1
1	A	9	CYS	HB3	3.342	0.011	2
1	A	9	CYS	HB2	2.886	0.014	2
1	A	110	HIS	HA	4.476	0.015	1
1	A	110	HIS	HB3	2.481	0.002	2
1	A	110	HIS	HB2	2.6	0.01	2
1	A	78	HIS	HB3	2.643	0.015	2
1	A	78	HIS	HB2	2.931	0.01	2
1	A	78	HIS	HA	4.039	0.011	1
1	A	106	HIS	HB3	2.9	0.01	2
1	A	106	HIS	HB2	2.703	0.011	2
1	A	106	HIS	N	118.237	0.053	1
1	A	22	HIS	HA	4.167	0.01	1
1	A	22	HIS	HB3	2.858	0.011	2
1	A	22	HIS	HB2	2.715	0.011	2
1	A	96	GLN	HA	4.845	0.011	1
1	A	97	PHE	HA	4.456	0.014	1
1	A	97	PHE	HB3	3.114	0.011	2
1	A	88	TYR	HA	4.453	0.014	1
1	A	88	TYR	HB2	2.763	0.011	1
1	A	88	TYR	HB3	2.764	0.011	1
1	A	108	ARG	HA	4.002	0.009	1
1	A	108	ARG	HB2	1.614	0.008	1
1	A	108	ARG	HB3	1.614	0.008	1
1	A	105	ARG	HB2	1.64	0.011	1
1	A	105	ARG	HB3	1.639	0.011	1
1	A	100	PRO	HA	3.463	0.014	1
1	A	103	LEU	HB2	1.706	0.013	2
1	A	103	LEU	HB3	1.029	0.009	2
1	A	103	LEU	HD21	0.864	0.015	2
1	A	103	LEU	HD22	0.864	0.015	2
1	A	103	LEU	HD23	0.864	0.015	2
1	A	103	LEU	HD11	0.775	0.01	2
1	A	103	LEU	HD12	0.775	0.01	2
1	A	103	LEU	HD13	0.775	0.01	2
1	A	103	LEU	HG	1.429	0.01	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	83	SER	HA	4.261	0.01	1
1	A	83	SER	HB2	3.775	0.012	1
1	A	83	SER	HB3	3.775	0.012	1
1	A	81	ILE	HA	3.798	0.006	1
1	A	80	ARG	HA	3.936	0.011	1
1	A	80	ARG	HB2	1.677	0.008	1
1	A	80	ARG	HB3	1.677	0.008	1
1	A	80	ARG	HG3	1.54	0.012	1
1	A	80	ARG	HG2	1.54	0.012	1
1	A	77	ARG	HB2	1.692	0.014	1
1	A	77	ARG	HB3	1.692	0.014	1
1	A	77	ARG	HA	3.799	0.008	1
1	A	97	PHE	HD1	7.039	0.012	3
1	A	97	PHE	HD2	7.039	0.012	3
1	A	8	TYR	HD1	6.692	0.013	3
1	A	8	TYR	HD2	6.692	0.013	3
1	A	13	PHE	HD1	7.02	0.012	3
1	A	13	PHE	HD2	7.02	0.012	3
1	A	4	TYR	HD1	6.888	0.01	3
1	A	4	TYR	HD2	6.888	0.01	3
1	A	21	ARG	HB3	1.648	0.015	1
1	A	21	ARG	HB2	1.648	0.015	1
1	A	21	ARG	HG2	1.513	0.01	1
1	A	21	ARG	HG3	1.513	0.01	1
1	A	103	LEU	CD1	23.066	0.038	2
1	A	3	PRO	HG3	1.693	0.01	1
1	A	108	ARG	HG2	1.515	0.01	1
1	A	108	ARG	HG3	1.515	0.01	1
1	A	105	ARG	HG3	1.332	0.008	1
1	A	105	ARG	HG2	1.332	0.008	1
1	A	77	ARG	HG2	1.439	0.009	1
1	A	77	ARG	HG3	1.439	0.009	1
1	A	77	ARG	HD2	3.057	0.012	1
1	A	77	ARG	HD3	3.057	0.012	1
1	A	80	ARG	HD3	3.053	0.01	1
1	A	80	ARG	HD2	3.053	0.01	1
1	A	61	LYS	HA	4.907	0.014	1
1	A	69	PHE	HD1	7.04	0.011	3
1	A	69	PHE	HD2	7.04	0.011	3
1	A	78	HIS	HD2	6.719	0.015	1
1	A	64	GLU	HA	4.075	0.012	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	21	ARG	HA	3.905	0.008	1
1	A	21	ARG	HD2	2.995	0.015	1
1	A	21	ARG	HD3	2.995	0.015	1
1	A	64	GLU	HB3	1.008	0.004	2
1	A	64	GLU	HB2	1.186	0.009	2
1	A	64	GLU	HG2	1.675	0.014	1
1	A	64	GLU	HG3	1.675	0.014	1
1	A	67	LYS	HG2	0.923	0.014	1
1	A	67	LYS	HG3	0.923	0.014	1
1	A	75	LEU	HB2	1.041	0.015	2
1	A	76	LYS	HA	3.648	0.008	1
1	A	59	PRO	HD3	3.483	0.009	1
1	A	59	PRO	HD2	3.483	0.009	1
1	A	68	GLN	HG2	2.037	0.011	1
1	A	68	GLN	HG3	2.037	0.011	1
1	A	59	PRO	HA	4.352	0.0	1
1	A	59	PRO	HB2	2.093	0.008	1
1	A	59	PRO	HB3	2.093	0.008	1
1	A	59	PRO	HG3	1.822	0.014	1
1	A	59	PRO	HG2	1.822	0.014	1
1	A	68	GLN	HA	4.678	0.011	1
1	A	61	LYS	HE3	2.782	0.012	1
1	A	61	LYS	HE2	2.782	0.012	1
1	A	61	LYS	HG2	0.973	0.012	1
1	A	61	LYS	HG3	0.973	0.012	1
1	A	61	LYS	HB3	1.431	0.013	1
1	A	61	LYS	HB2	1.431	0.013	1
1	A	61	LYS	HD3	1.427	0.011	1
1	A	61	LYS	HD2	1.427	0.011	1
1	A	69	PHE	HB3	2.54	0.015	2
1	A	69	PHE	HB2	3.121	0.009	2
1	A	75	LEU	HG	1.346	0.007	1
1	A	75	LEU	CG	26.908	0.021	1
1	A	76	LYS	HE2	2.78	0.011	1
1	A	76	LYS	HE3	2.78	0.011	1
1	A	76	LYS	HB3	1.721	0.014	1
1	A	76	LYS	HB2	1.721	0.014	1
1	A	76	LYS	HG2	1.233	0.012	1
1	A	76	LYS	HG3	1.232	0.012	1
1	A	76	LYS	HD3	1.487	0.013	1
1	A	76	LYS	HD2	1.487	0.013	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	81	ILE	HG21	0.443	0.011	1
1	A	81	ILE	HG22	0.443	0.011	1
1	A	81	ILE	HG23	0.443	0.011	1
1	A	81	ILE	HD11	0.564	0.014	1
1	A	81	ILE	HD12	0.564	0.014	1
1	A	81	ILE	HD13	0.564	0.014	1
1	A	82	HIS	HB3	2.951	0.01	2
1	A	82	HIS	HB2	3.196	0.008	2
1	A	82	HIS	HA	4.627	0.005	1
1	A	87	PRO	HD3	3.451	0.009	1
1	A	87	PRO	HD2	3.451	0.009	1
1	A	87	PRO	HB2	1.871	0.014	1
1	A	87	PRO	HB3	1.871	0.014	1
1	A	87	PRO	HG3	1.677	0.007	1
1	A	87	PRO	HG2	1.677	0.007	1
1	A	68	GLN	HB3	1.738	0.004	2
1	A	68	GLN	HB2	1.603	0.01	2
1	A	81	ILE	HG13	0.786	0.011	1
1	A	78	HIS	CD2	130.741	.	1
1	A	81	ILE	HB	1.536	0.01	1
1	A	81	ILE	HG12	0.786	0.011	1
1	A	82	HIS	HD2	6.516	0.008	1
1	A	82	HIS	CD2	130.548	0.028	1
1	A	82	HIS	HE1	7.882	0.011	1
1	A	82	HIS	CE1	142.545	0.07	1
1	A	78	HIS	HE1	7.9	0.003	1
1	A	78	HIS	CE1	142.456	.	1
1	A	69	PHE	CD1	135.014	0.033	3
1	A	69	PHE	CD2	135.014	0.033	3
1	A	105	ARG	HD3	3.062	0.008	1
1	A	105	ARG	HD2	3.062	0.008	1
1	A	105	ARG	HA	3.815	0.009	1
1	A	103	LEU	HA	2.975	0.008	1
1	A	97	PHE	HB2	2.596	0.009	2
1	A	96	GLN	HG2	2.189	0.012	1
1	A	96	GLN	HG3	2.189	0.012	1
1	A	96	GLN	HB3	2.034	0.014	1
1	A	96	GLN	HB2	2.034	0.014	1
1	A	92	HIS	HB3	2.205	0.013	2
1	A	91	ILE	HA	3.915	0.01	1
1	A	91	ILE	HB	1.7	0.007	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	91	ILE	HG12	0.957	0.012	1
1	A	91	ILE	HG13	0.957	0.012	1
1	A	91	ILE	HG21	0.625	0.009	1
1	A	91	ILE	HG22	0.625	0.009	1
1	A	91	ILE	HG23	0.625	0.009	1
1	A	18	SER	HA	3.871	0.008	1
1	A	18	SER	HB3	3.799	0.013	1
1	A	18	SER	HB2	3.799	0.013	1
1	A	14	SER	HA	4.491	0.006	1
1	A	14	SER	HB2	3.94	0.013	1
1	A	14	SER	HB3	3.94	0.013	1
1	A	16	PRO	HD3	3.595	0.015	2
1	A	16	PRO	HD2	3.032	0.014	2
1	A	16	PRO	HB3	1.864	0.009	1
1	A	16	PRO	HB2	1.864	0.009	1
1	A	12	SER	HA	4.896	0.009	1
1	A	12	SER	HB2	3.486	0.009	1
1	A	12	SER	HB3	3.486	0.009	1
1	A	87	PRO	HA	4.165	0.011	1
1	A	19	LYS	HB3	1.593	0.014	2
1	A	19	LYS	HB2	1.396	0.014	2
1	A	19	LYS	HG2	0.997	0.008	1
1	A	19	LYS	HG3	0.997	0.008	1
1	A	26	HIS	HA	4.467	.	1
1	A	86	LYS	HA	4.391	0.012	1
1	A	86	LYS	HB2	1.44	0.013	1
1	A	86	LYS	HB3	1.44	0.013	1
1	A	86	LYS	HD3	1.207	0.014	1
1	A	86	LYS	HD2	1.207	0.014	1
1	A	86	LYS	HG2	1.069	0.007	1
1	A	86	LYS	HG3	1.069	0.007	1
1	A	88	TYR	HD1	6.883	0.01	3
1	A	88	TYR	HD2	6.883	0.01	3
1	A	92	HIS	HB2	1.768	0.013	2
1	A	108	ARG	HD2	3.048	0.007	1
1	A	108	ARG	HD3	3.048	0.007	1
1	A	8	TYR	HB2	1.752	0.01	2
1	A	18	SER	CB	61.877	0.016	1
1	A	19	LYS	HE3	2.793	0.012	1
1	A	19	LYS	HE2	2.793	0.012	1
1	A	4	TYR	CD1	135.925	0.069	3

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	TYR	CD2	135.925	0.069	3
1	A	4	TYR	HE1	6.702	0.001	3
1	A	4	TYR	HE2	6.702	0.001	3
1	A	8	TYR	CD1	135.572	0.061	3
1	A	8	TYR	CD2	135.572	0.061	3
1	A	26	HIS	CD2	130.448	0.078	1
1	A	26	HIS	HB3	2.656	0.012	2
1	A	26	HIS	HB2	2.48	0.006	2
1	A	22	HIS	HD2	6.966	0.004	1
1	A	22	HIS	CD2	130.823	0.0	1
1	A	26	HIS	HE1	7.922	0.006	1
1	A	26	HIS	CE1	142.848	0.001	1
1	A	91	ILE	HD11	0.749	0.007	1
1	A	91	ILE	HD12	0.749	0.007	1
1	A	91	ILE	HD13	0.749	0.007	1
1	A	106	HIS	HD2	6.681	0.004	1
1	A	88	TYR	CD1	136.067	0.026	3
1	A	88	TYR	CD2	136.067	0.026	3
1	A	97	PHE	CD1	135.172	0.041	3
1	A	97	PHE	CD2	135.172	0.041	3
1	A	97	PHE	HZ	5.869	0.005	1
1	A	8	TYR	HE1	6.649	0.004	3
1	A	8	TYR	HE2	6.649	0.004	3
1	A	8	TYR	CE1	121.095	0.057	3
1	A	8	TYR	CE2	121.095	0.057	3
1	A	26	HIS	HD2	6.443	0.006	1
1	A	16	PRO	HA	3.556	0.011	1
1	A	19	LYS	HA	2.613	0.007	1
1	A	13	PHE	CD1	134.878	0.06	3
1	A	13	PHE	CD2	134.878	0.06	3
1	A	97	PHE	HE1	6.665	0.002	3
1	A	97	PHE	HE2	6.665	0.002	3
1	A	97	PHE	CZ	131.433	0.017	1
1	A	106	HIS	HE1	7.878	.	1
1	A	13	PHE	CZ	131.642	0.0	1
1	A	13	PHE	HZ	5.872	0.004	1
1	A	110	HIS	CD2	131.677	0.047	1
1	A	110	HIS	HD2	6.574	0.009	1
1	A	110	HIS	HE1	7.913	.	1
1	A	69	PHE	CZ	131.475	.	1
1	A	69	PHE	HZ	5.878	0.001	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
$^{13}C_{\alpha}$	103	-0.16 ± 0.16	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	95	0.25 ± 0.17	None needed (< 0.5 ppm)
$^{13}C'$	94	0.15 ± 0.16	None needed (< 0.5 ppm)
^{15}N	95	1.02 ± 0.77	None needed (imprecise)

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 76%, i.e. 251 atoms were assigned a chemical shift out of a possible 332. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	102/119 (86%)	38/48 (79%)	43/48 (90%)	21/23 (91%)
Sidechain	134/181 (74%)	87/117 (74%)	47/57 (82%)	0/7 (0%)
Aromatic	15/32 (47%)	8/17 (47%)	7/11 (64%)	0/4 (0%)
Overall	251/332 (76%)	133/182 (73%)	97/116 (84%)	21/34 (62%)

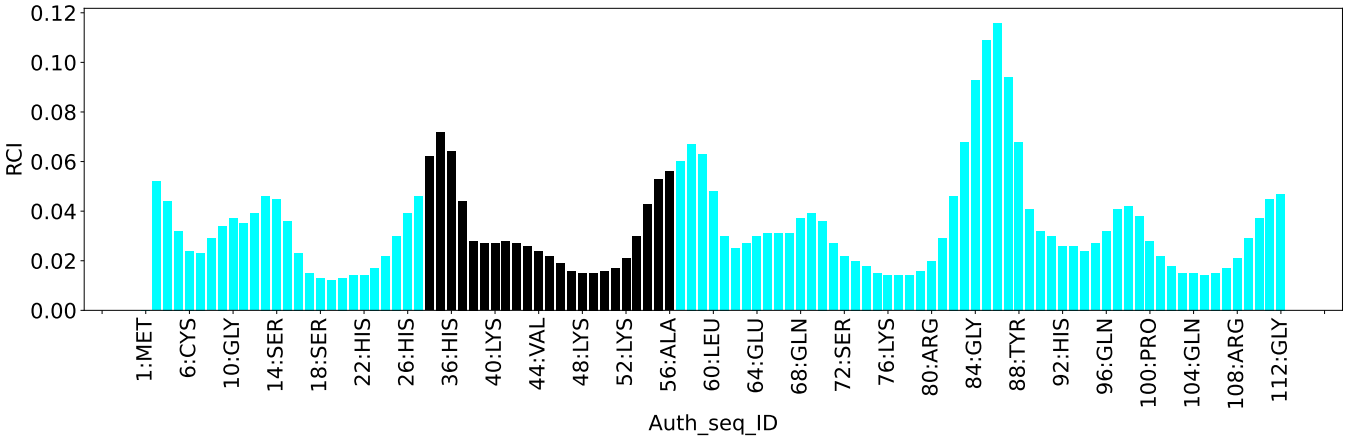
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.12
0.10
0.08
0.06
0.04
0.02
0.00
1:MET
6:CYS
10:GLY
14:SER
18:SER
22:HIS
26:HIS
36:HIS
40:LYS
44:VAL
48:LYS
52:LYS
56:ALA
60:LEU
64:GLU
68:GLN
72:SER
76:LYS
80:ARG
84:GLY
88:TYR
92:HIS
96:GLN
100:PRO
104:GLN
108:ARG
112:GLY
Auth_seq_ID

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	265
Intra-residue (|i-j|=0)	133
Sequential (|i-j|=1)	76
Medium range (|i-j|>1 and |i-j|<5)	54
Long range (|i-j|≥5)	2
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	51
Number of unmapped restraints	0
Number of restraints per residue	2.8
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.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.3	0.13
0.2-0.5 (Medium)	0.1	0.36
>0.5 (Large)	0.2	0.95

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	2.9	5.6
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

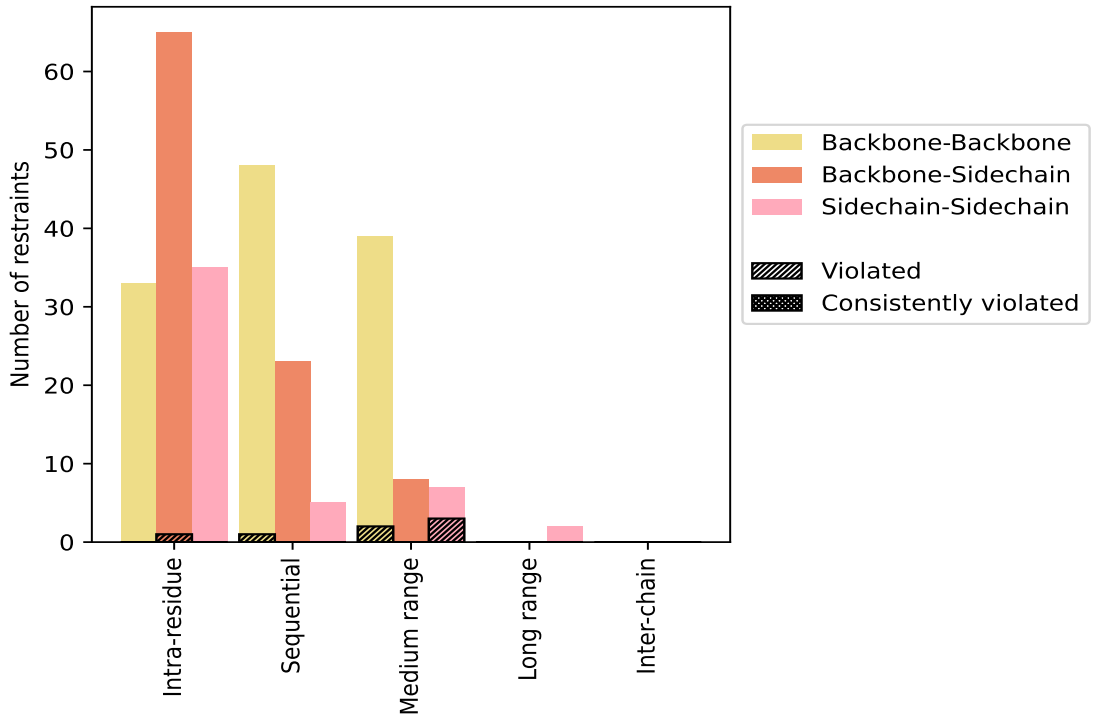
9.1 Summary of distance violations (i)

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)	133	50.2	1	0.8	0.4	0	0.0	0.0
Backbone-Backbone	33	12.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	65	24.5	1	1.5	0.4	0	0.0	0.0
Sidechain-Sidechain	35	13.2	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	76	28.7	1	1.3	0.4	0	0.0	0.0
Backbone-Backbone	48	18.1	1	2.1	0.4	0	0.0	0.0
Backbone-Sidechain	23	8.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	5	1.9	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	54	20.4	5	9.3	1.9	0	0.0	0.0
Backbone-Backbone	39	14.7	2	5.1	0.8	0	0.0	0.0
Backbone-Sidechain	8	3.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	7	2.6	3	42.9	1.1	0	0.0	0.0
Long range (|i-j|≥5)	2	0.8	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	2	0.8	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	0	0.0	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	265	100.0	7	2.6	2.6	0	0.0	0.0
Backbone-Backbone	120	45.3	3	2.5	1.1	0	0.0	0.0
Backbone-Sidechain	96	36.2	1	1.0	0.4	0	0.0	0.0
Sidechain-Sidechain	49	18.5	3	6.1	1.1	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

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	1	0	0	1	0.29	0.29	0.0	0.29
3	0	0	2	0	0	2	0.41	0.69	0.28	0.41
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0	0	0	0.0	0.0	0.0	0.0
7	1	0	0	0	0	1	0.36	0.36	0.0	0.36
8	0	0	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	3	0	0	3	0.11	0.12	0.0	0.11
10	0	0	1	0	0	1	0.57	0.57	0.0	0.57
11	0	1	0	0	0	1	0.11	0.11	0.0	0.11

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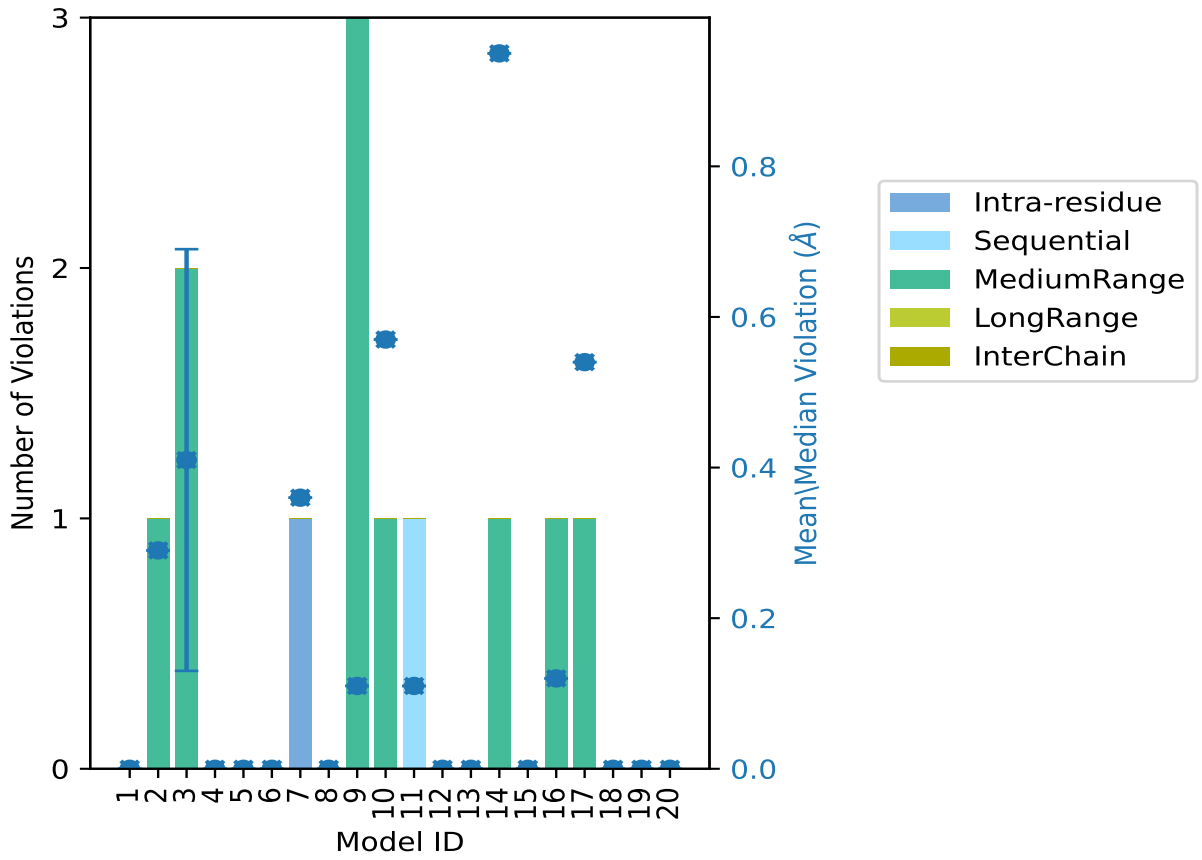
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	1	0	0	1	0.95	0.95	0.0	0.95
15	0	0	0	0	0	0	0.0	0.0	0.0	0.0
16	0	0	1	0	0	1	0.12	0.12	0.0	0.12
17	0	0	1	0	0	1	0.54	0.54	0.0	0.54
18	0	0	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0	0	0	0.0	0.0	0.0	0.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

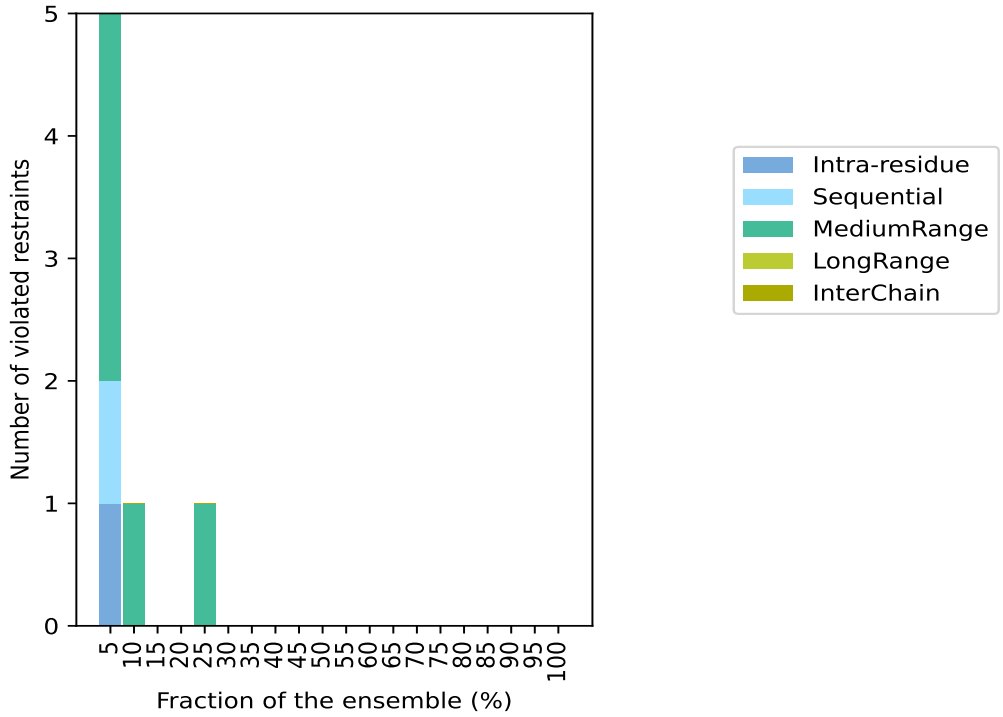
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 258(IR:132, SQ:75, MR:49, LR:2, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
1	1	3	0	0	5	1	5.0
0	0	1	0	0	1	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	1	0	0	1	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

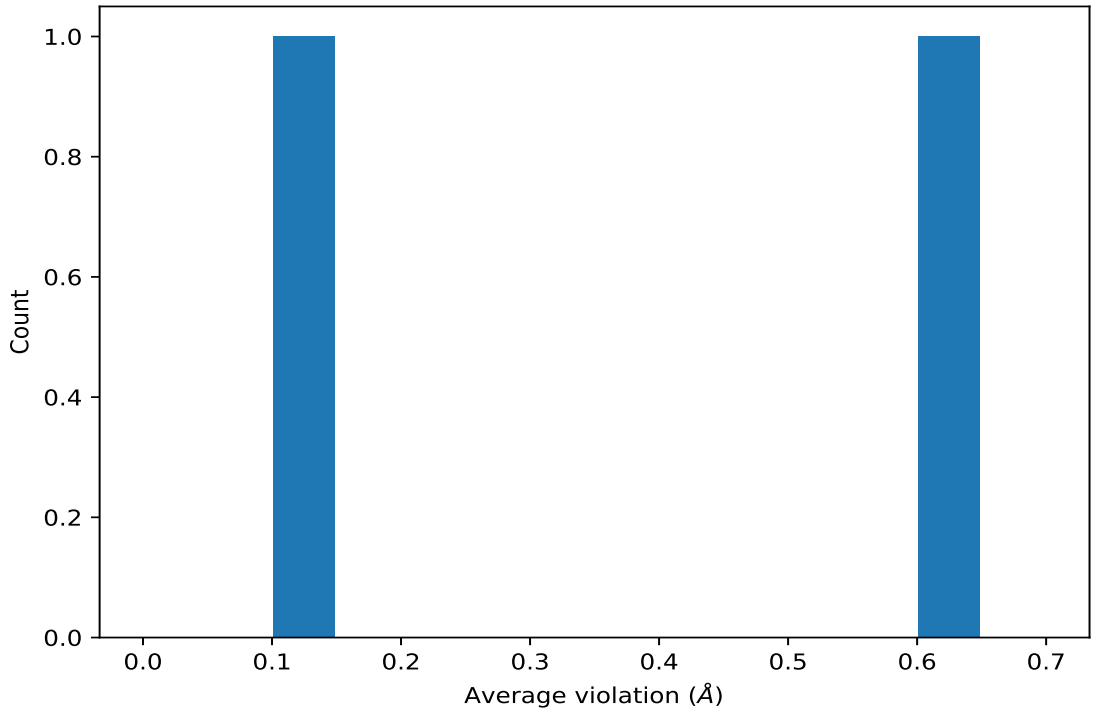
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

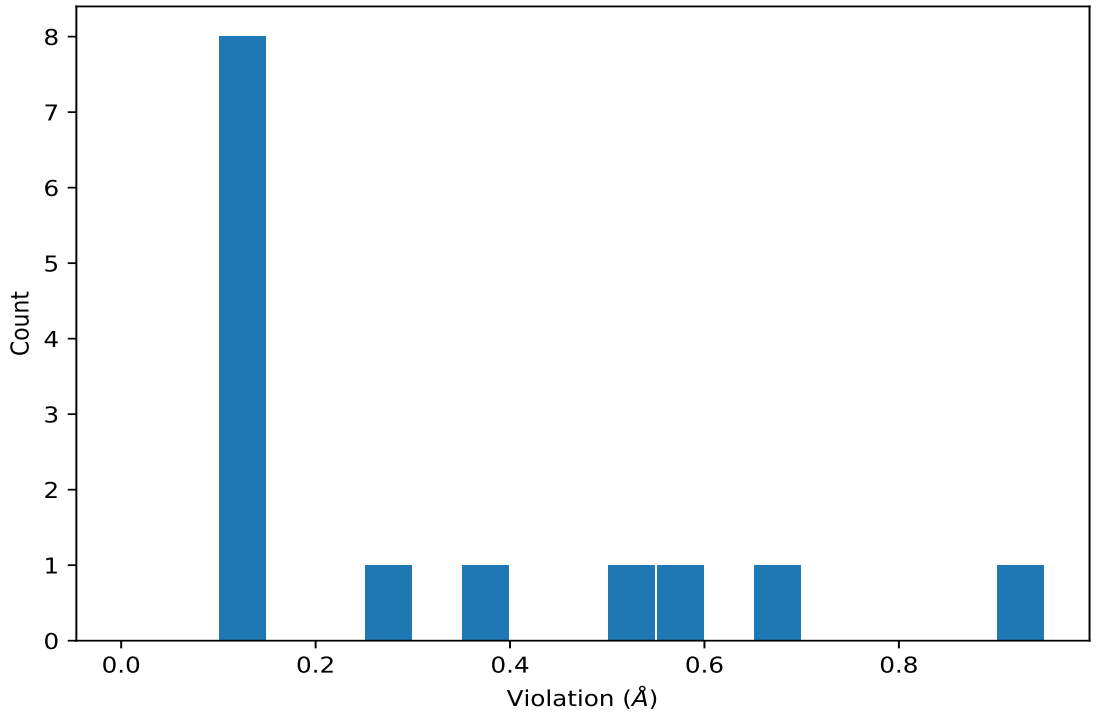
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,53)	1:A:41:PHE:HZ	1:A:39:LYS:HE2	5	0.61	0.21	0.57
(1,113)	1:A:51:LEU:H	1:A:48:LYS:HA	2	0.12	0.01	0.12

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations (i)

The following table provides the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:A:41:PHE:HZ	1:A:39:LYS:HE2	14	0.95
(1,53)	1:A:41:PHE:HZ	1:A:39:LYS:HE2	3	0.69
(1,53)	1:A:41:PHE:HZ	1:A:39:LYS:HE2	10	0.57
(1,53)	1:A:41:PHE:HZ	1:A:39:LYS:HE2	17	0.54
(1,174)	1:A:55:ILE:H	1:A:55:ILE:HG12	7	0.36
(1,53)	1:A:41:PHE:HZ	1:A:39:LYS:HE2	2	0.29
(1,113)	1:A:51:LEU:H	1:A:48:LYS:HA	3	0.13
(1,45)	1:A:50:HIS:HB3	1:A:53:ILE:HG21	16	0.12
(1,45)	1:A:50:HIS:HB3	1:A:53:ILE:HG22	16	0.12
(1,45)	1:A:50:HIS:HB3	1:A:53:ILE:HG23	16	0.12
(1,41)	1:A:50:HIS:HB3	1:A:47:LEU:HG	9	0.12
(1,70)	1:A:56:ALA:H	1:A:57:ASP:HA	11	0.11

10 Dihedral-angle violation analysis

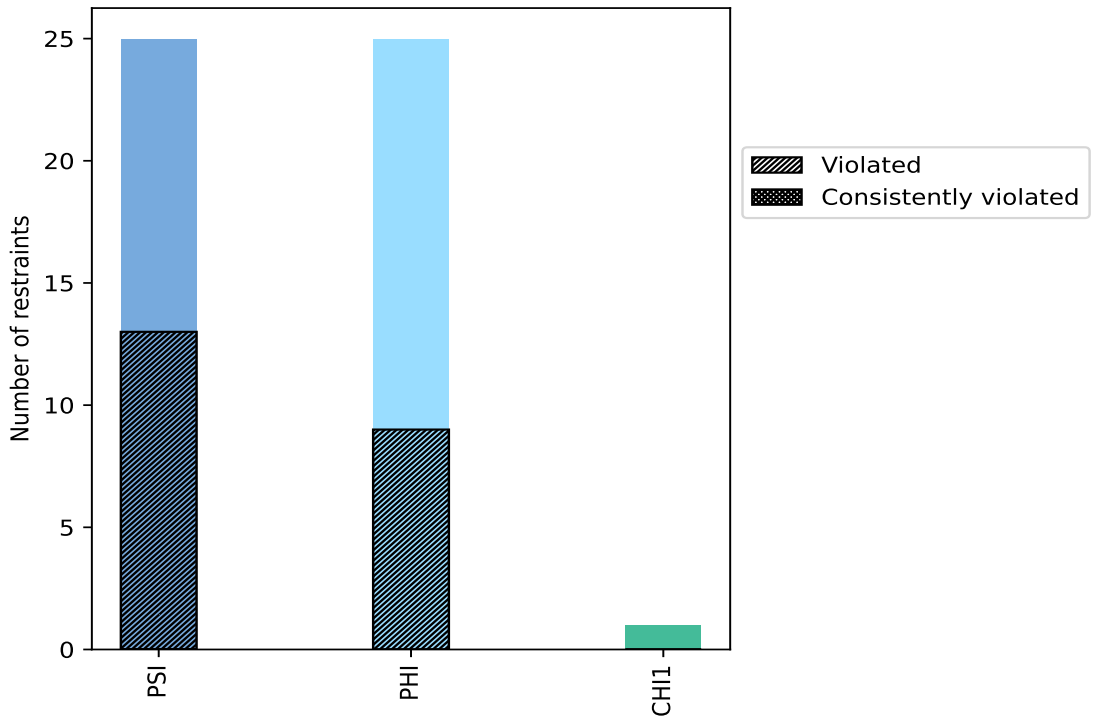
10.1 Summary of dihedral-angle violations

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	25	49.0	13	52.0	25.5	0	0.0	0.0
PHI	25	49.0	9	36.0	17.6	0	0.0	0.0
CHI1	1	2.0	0	0.0	0.0	0	0.0	0.0
Total	51	100.0	22	43.1	43.1	0	0.0	0.0

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations



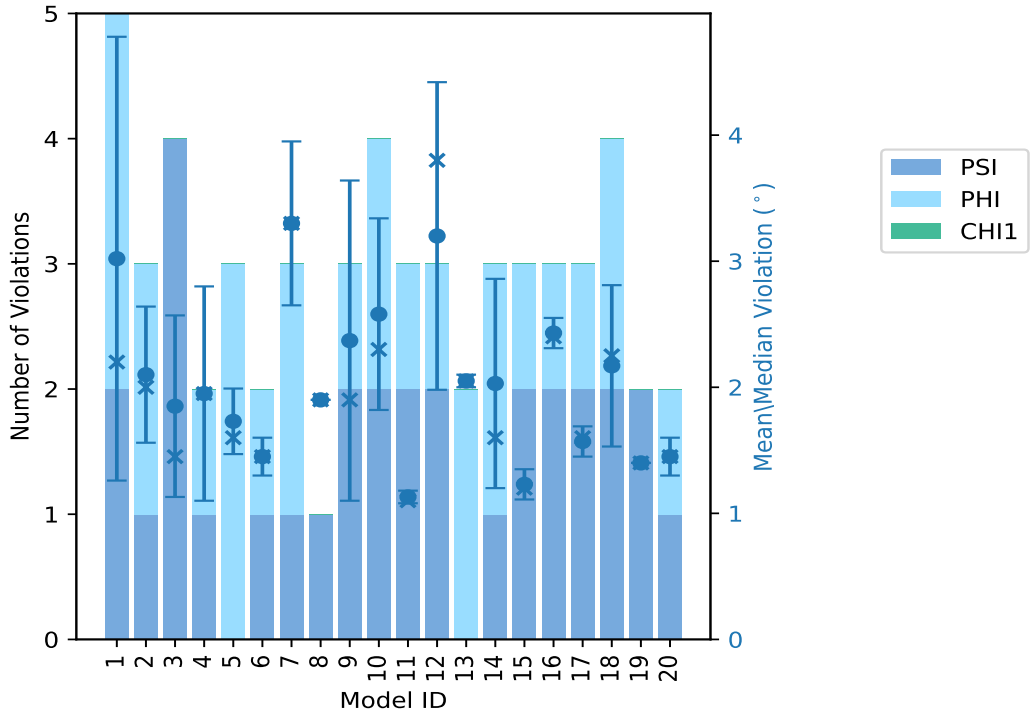
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations				Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	CHI1	Total				
1	2	3	0	5	3.02	5.6	1.76	2.2
2	1	2	0	3	2.1	2.8	0.54	2.0
3	4	0	0	4	1.85	3.1	0.72	1.45
4	1	1	0	2	1.95	2.8	0.85	1.95
5	0	3	0	3	1.73	2.1	0.26	1.6
6	1	1	0	2	1.45	1.6	0.15	1.45
7	1	2	0	3	3.3	4.1	0.65	3.3
8	1	0	0	1	1.9	1.9	0.0	1.9
9	2	1	0	3	2.37	4.1	1.27	1.9
10	2	2	0	4	2.58	3.8	0.76	2.3
11	2	1	0	3	1.13	1.2	0.05	1.1
12	2	1	0	3	3.2	4.3	1.22	3.8
13	0	2	0	2	2.05	2.1	0.05	2.05
14	1	2	0	3	2.03	3.2	0.83	1.6
15	2	1	0	3	1.23	1.4	0.12	1.2
16	2	1	0	3	2.43	2.6	0.12	2.4
17	2	1	0	3	1.57	1.7	0.12	1.6
18	2	2	0	4	2.17	3.0	0.64	2.25
19	2	0	0	2	1.4	1.4	0.0	1.4
20	1	1	0	2	1.45	1.6	0.15	1.45

10.2.1 Bar graph : Dihedral violation statistics for each model (i)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

10.3 Dihedral-angle violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints				Fraction of the ensemble	
PSI	PHI	CHI1	Total	Count[1]	%
6	4	0	10	1	5.0
3	3	0	6	2	10.0
1	0	0	1	3	15.0
0	1	0	1	4	20.0
2	0	0	2	5	25.0
1	0	0	1	6	30.0
0	0	0	0	7	35.0
0	0	0	0	8	40.0
0	0	0	0	9	45.0
0	0	0	0	10	50.0
0	0	0	0	11	55.0

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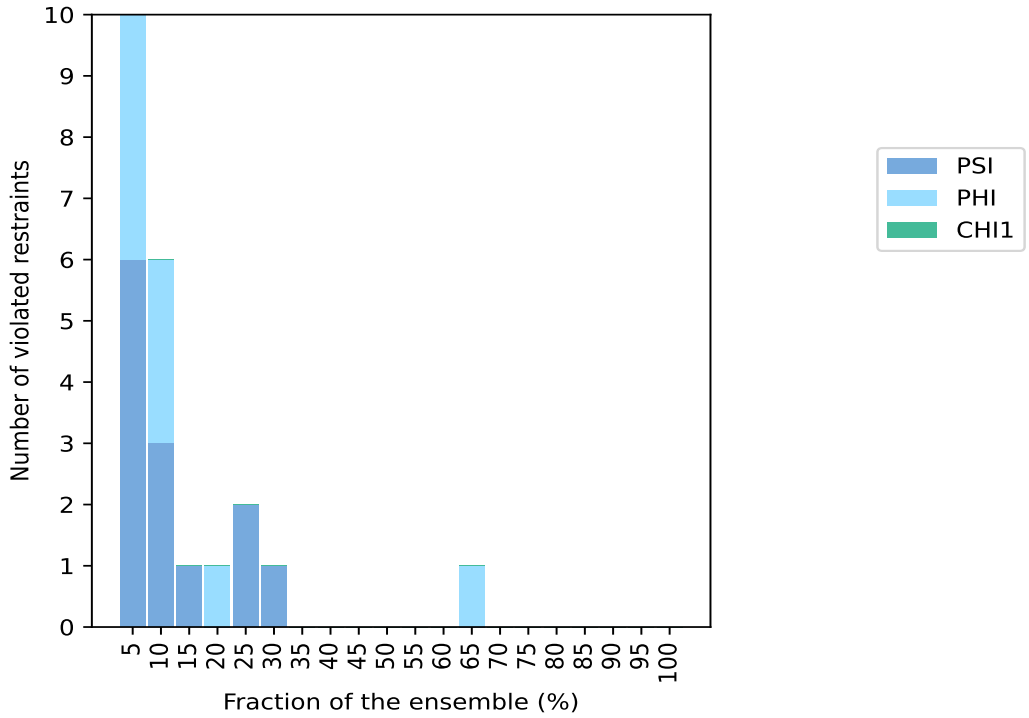
Number of violated restraints				Fraction of the ensemble	
PSI	PHI	CHI1	Total	Count[1]	%
0	0	0	0	12	60.0
0	1	0	1	13	65.0
0	0	0	0	14	70.0
0	0	0	0	15	75.0
0	0	0	0	16	80.0
0	0	0	0	17	85.0
0	0	0	0	18	90.0
0	0	0	0	19	95.0
0	0	0	0	20	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble

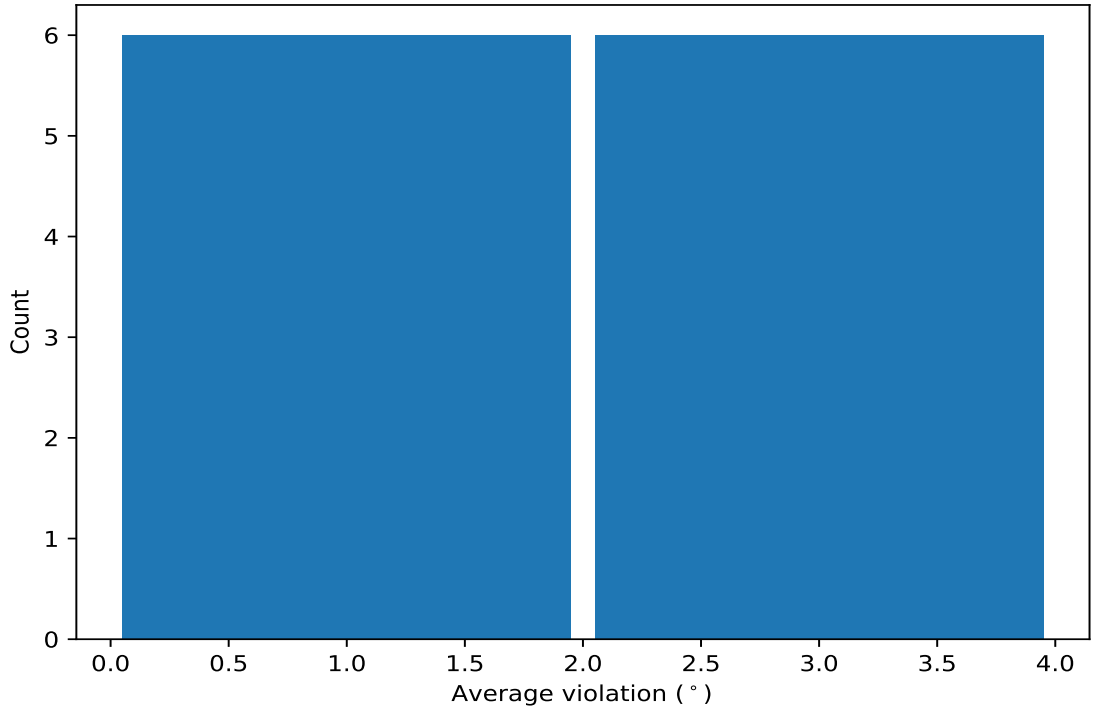


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

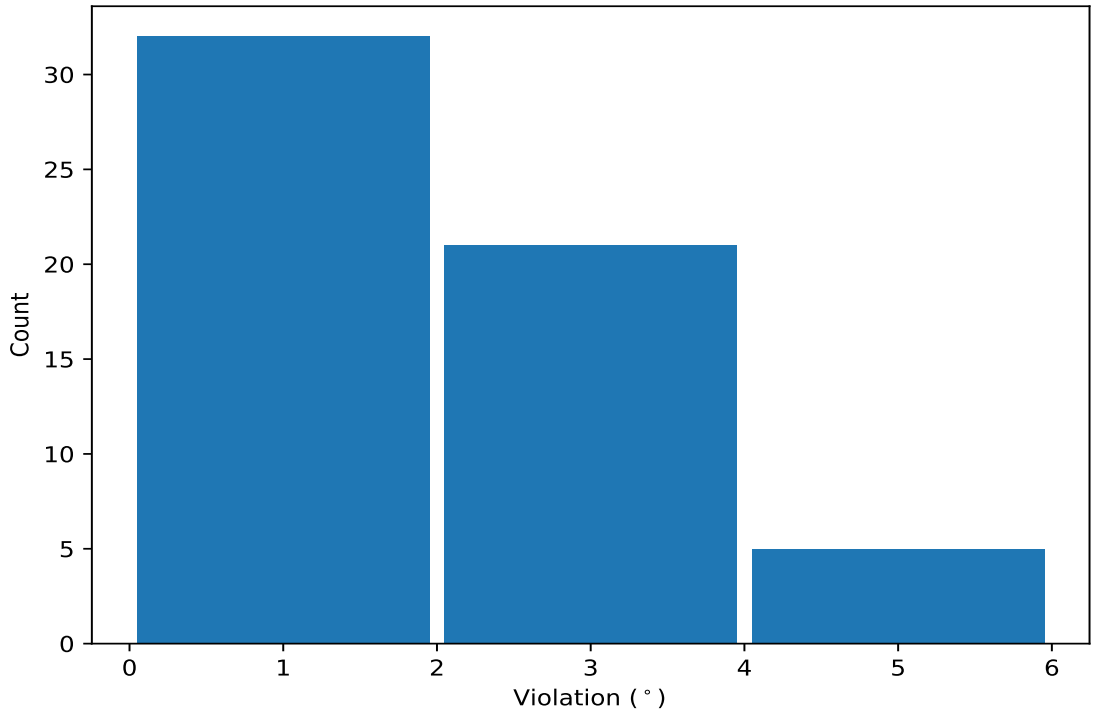
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,26)	1:A:44:VAL:C	1:A:45:GLY:N	1:A:45:GLY:CA	1:A:45:GLY:C	13	2.48	0.91	2.4
(1,27)	1:A:45:GLY:N	1:A:45:GLY:CA	1:A:45:GLY:C	1:A:46:ASN:N	6	2.47	0.86	2.3
(1,25)	1:A:44:VAL:N	1:A:44:VAL:CA	1:A:44:VAL:C	1:A:45:GLY:N	5	2.24	0.93	2.2
(1,6)	1:A:33:LYS:N	1:A:33:LYS:CA	1:A:33:LYS:C	1:A:34:CYS:N	5	1.38	0.17	1.4
(1,48)	1:A:55:ILE:C	1:A:56:ALA:N	1:A:56:ALA:CA	1:A:56:ALA:C	4	3.38	1.59	3.2
(1,29)	1:A:46:ASN:N	1:A:46:ASN:CA	1:A:46:ASN:C	1:A:47:LEU:N	3	1.23	0.12	1.2
(1,47)	1:A:55:ILE:N	1:A:55:ILE:CA	1:A:55:ILE:C	1:A:56:ALA:N	2	3.95	0.65	3.95
(1,13)	1:A:38:ASP:N	1:A:38:ASP:CA	1:A:38:ASP:C	1:A:39:LYS:N	2	2.25	0.85	2.25
(1,10)	1:A:35:PRO:C	1:A:36:HIS:N	1:A:36:HIS:CA	1:A:36:HIS:C	2	1.7	0.2	1.7
(1,11)	1:A:36:HIS:N	1:A:36:HIS:CA	1:A:36:HIS:C	1:A:37:CYS:N	2	1.7	0.3	1.7

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints

The following table provides the list of violationsfor the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,48)	1:A:55:ILE:C	1:A:56:ALA:N	1:A:56:ALA:CA	1:A:56:ALA:C	1	5.6
(1,47)	1:A:55:ILE:N	1:A:55:ILE:CA	1:A:55:ILE:C	1:A:56:ALA:N	1	4.6
(1,26)	1:A:44:VAL:C	1:A:45:GLY:N	1:A:45:GLY:CA	1:A:45:GLY:C	12	4.3
(1,48)	1:A:55:ILE:C	1:A:56:ALA:N	1:A:56:ALA:CA	1:A:56:ALA:C	7	4.1
(1,27)	1:A:45:GLY:N	1:A:45:GLY:CA	1:A:45:GLY:C	1:A:46:ASN:N	9	4.1
(1,26)	1:A:44:VAL:C	1:A:45:GLY:N	1:A:45:GLY:CA	1:A:45:GLY:C	10	3.8
(1,25)	1:A:44:VAL:N	1:A:44:VAL:CA	1:A:44:VAL:C	1:A:45:GLY:N	12	3.8
(1,47)	1:A:55:ILE:N	1:A:55:ILE:CA	1:A:55:ILE:C	1:A:56:ALA:N	7	3.3
(1,26)	1:A:44:VAL:C	1:A:45:GLY:N	1:A:45:GLY:CA	1:A:45:GLY:C	14	3.2
(1,13)	1:A:38:ASP:N	1:A:38:ASP:CA	1:A:38:ASP:C	1:A:39:LYS:N	3	3.1