wwPDB NMR Structure Validation Summary Report

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BMRB ID	:	18806
Title	:	Solution Structure of Miz-1 zinc finger 7
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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:

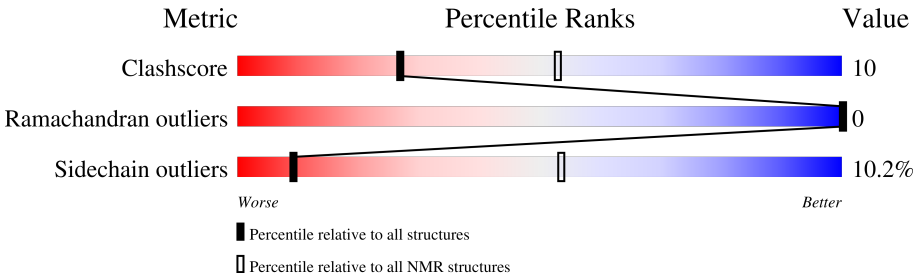
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 85%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	112	16% . . . 74%

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 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:60-A:83 (24)	0.35	15

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 6 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 464 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	463	139	235	48	39	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 (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	1	1	1

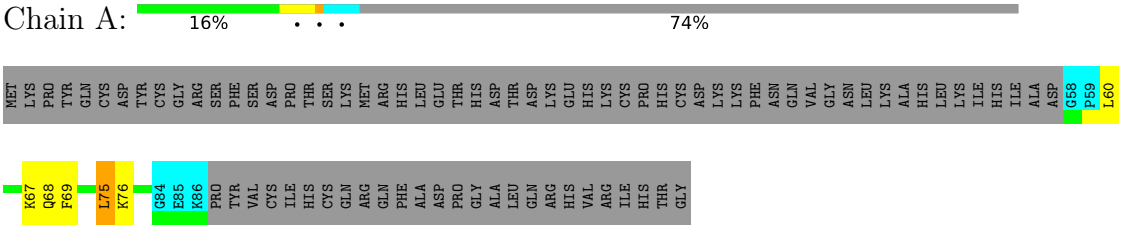
4 Residue-property plots

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:

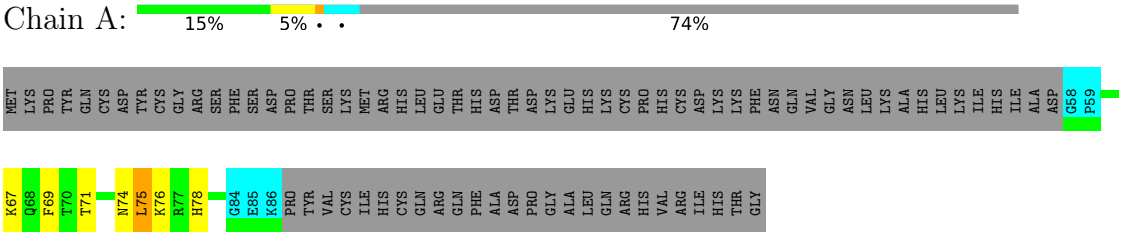


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 15. 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	342
Number of unparsed shifts	0
Number of shifts with mapping errors	844
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

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	195	203	203	4±2
All	All	3920	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 44 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LEU:HB3	1:A:75:LEU:HD12	0.78	1.53	13	1
1:A:61:LYS:HA	1:A:68:GLN:HA	0.76	1.54	20	4
1:A:62:CYS:SG	1:A:78:HIS:CD2	0.73	2.82	13	1
1:A:64:GLU:CD	1:A:64:GLU:H	0.64	1.99	13	1
1:A:69:PHE:CD1	1:A:75:LEU:HG	0.61	2.30	13	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	24/112 (21%)	24±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	480/2240 (21%)	480 (100%)	0 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	22/100 (22%)	20±1 (90±4%)	2±1 (10±4%)	9	53
All	All	440/2000 (22%)	395 (90%)	45 (10%)	9	53

5 of 7 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	75	LEU	17
1	A	76	LYS	13
1	A	67	LYS	9
1	A	71	THR	3
1	A	80	ARG	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.6 Ligand geometry (i)

Of 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 85% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping

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

Total number of shifts	1186
Number of shifts mapped to atoms	342
Number of unparsed shifts	0
Number of shifts with mapping errors	844
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 844) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
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	1	MET	CE	19.935	0.024	1
1	A	3	PRO	HA	4.147	0.006	1
1	A	3	PRO	HB2	1.312	0.009	2
1	A	3	PRO	HB3	1.923	0.01	2
1	A	3	PRO	HD2	3.477	0.012	2
1	A	3	PRO	HD3	3.614	0.01	2
1	A	3	PRO	HG2	1.693	0.01	1
1	A	3	PRO	HG3	1.693	0.01	1
1	A	3	PRO	C	176.083	.	1
1	A	3	PRO	CA	63.415	0.077	1
1	A	3	PRO	CB	31.877	0.043	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	PRO	CD	50.236	.	1
1	A	3	PRO	CG	27.125	.	1
1	A	4	TYR	H	7.959	0.008	1
1	A	4	TYR	HA	4.46	0.013	1
1	A	4	TYR	HB2	2.651	0.013	2
1	A	4	TYR	HB3	2.825	0.012	2
1	A	4	TYR	HD1	6.888	0.01	3
1	A	4	TYR	HD2	6.888	0.01	3
1	A	4	TYR	HE1	6.702	0.001	3
1	A	4	TYR	HE2	6.702	0.001	3
1	A	4	TYR	C	174.569	.	1
1	A	4	TYR	CA	56.77	0.044	1
1	A	4	TYR	CB	38.43	0.058	1
1	A	4	TYR	CD1	135.925	0.069	3
1	A	4	TYR	CD2	135.925	0.069	3
1	A	4	TYR	N	117.838	0.034	1
1	A	5	GLN	H	8.544	0.008	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	HG2	2.02	0.015	1
1	A	5	GLN	HG3	2.02	0.015	1
1	A	5	GLN	C	175.122	.	1
1	A	5	GLN	CA	54.558	0.078	1
1	A	5	GLN	CB	31.592	0.062	1
1	A	5	GLN	CG	33.813	0.038	1
1	A	5	GLN	N	123.036	0.04	1
1	A	6	CYS	H	9.125	0.011	1
1	A	6	CYS	HA	4.277	0.014	1
1	A	6	CYS	HB2	3.368	0.012	2
1	A	6	CYS	HB3	2.863	0.013	2
1	A	6	CYS	C	176.578	.	1
1	A	6	CYS	CA	60.245	0.074	1
1	A	6	CYS	CB	30.278	0.048	1
1	A	6	CYS	N	125.821	0.031	1
1	A	7	ASP	H	8.738	0.014	1
1	A	7	ASP	HA	4.216	0.012	1
1	A	7	ASP	HB2	1.901	0.012	2
1	A	7	ASP	HB3	2.309	0.013	2
1	A	7	ASP	C	175.676	.	1
1	A	7	ASP	CA	56.35	0.063	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	ASP	CB	40.743	0.079	1
1	A	7	ASP	N	129.841	0.02	1
1	A	8	TYR	H	8.935	0.011	1
1	A	8	TYR	HA	4.24	0.007	1
1	A	8	TYR	HB2	1.752	0.01	2
1	A	8	TYR	HB3	2.384	0.014	2
1	A	8	TYR	HD1	6.692	0.013	3
1	A	8	TYR	HD2	6.692	0.013	3
1	A	8	TYR	HE1	6.649	0.004	3
1	A	8	TYR	HE2	6.649	0.004	3
1	A	8	TYR	C	176.44	.	1
1	A	8	TYR	CA	59.546	0.038	1
1	A	8	TYR	CB	38.06	0.079	1
1	A	8	TYR	CD1	135.572	0.061	3
1	A	8	TYR	CD2	135.572	0.061	3
1	A	8	TYR	CE1	121.095	0.057	3
1	A	8	TYR	CE2	121.095	0.057	3
1	A	8	TYR	N	119.023	0.036	1
1	A	9	CYS	H	8.105	0.009	1
1	A	9	CYS	HA	5.038	0.011	1
1	A	9	CYS	HB2	2.886	0.014	2
1	A	9	CYS	HB3	3.342	0.011	2
1	A	9	CYS	C	175.815	.	1
1	A	9	CYS	CA	58.31	0.043	1
1	A	9	CYS	CB	32.273	0.036	1
1	A	9	CYS	N	115.815	0.047	1
1	A	10	GLY	H	7.985	0.013	1
1	A	10	GLY	HA2	4.05	0.01	2
1	A	10	GLY	HA3	3.753	0.011	2
1	A	10	GLY	C	173.932	.	1
1	A	10	GLY	CA	46.039	0.043	1
1	A	10	GLY	N	111.402	0.04	1
1	A	11	ARG	H	7.928	0.008	1
1	A	11	ARG	HA	3.928	0.014	1
1	A	11	ARG	HB2	1.197	0.015	2
1	A	11	ARG	HB3	1.346	0.013	2
1	A	11	ARG	HD2	2.752	0.014	2
1	A	11	ARG	HD3	2.949	0.011	2
1	A	11	ARG	HG2	1.668	0.015	2
1	A	11	ARG	HG3	1.704	0.011	2
1	A	11	ARG	C	174.22	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	ARG	CA	57.602	0.011	1
1	A	11	ARG	CB	31.248	0.044	1
1	A	11	ARG	CD	43.278	0.019	1
1	A	11	ARG	CG	27.904	0.008	1
1	A	11	ARG	N	122.427	0.035	1
1	A	12	SER	H	7.89	0.011	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	12	SER	C	172.775	.	1
1	A	12	SER	CA	57.311	0.033	1
1	A	12	SER	CB	65.516	0.068	1
1	A	12	SER	N	115.605	0.048	1
1	A	13	PHE	H	8.392	0.01	1
1	A	13	PHE	HA	4.591	0.009	1
1	A	13	PHE	HB2	2.574	0.014	2
1	A	13	PHE	HB3	3.293	0.012	2
1	A	13	PHE	HD1	7.02	0.012	3
1	A	13	PHE	HD2	7.02	0.012	3
1	A	13	PHE	HZ	5.872	0.004	1
1	A	13	PHE	C	175.33	.	1
1	A	13	PHE	CA	57.369	0.03	1
1	A	13	PHE	CB	43.443	0.065	1
1	A	13	PHE	CD1	134.878	0.06	3
1	A	13	PHE	CD2	134.878	0.06	3
1	A	13	PHE	CZ	131.642	0.0	1
1	A	13	PHE	N	118.534	0.06	1
1	A	14	SER	H	9.09	0.003	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	14	SER	C	173.113	.	1
1	A	14	SER	CA	59.545	0.061	1
1	A	14	SER	CB	64.037	0.072	1
1	A	14	SER	N	114.545	0.046	1
1	A	15	ASP	H	7.443	0.007	1
1	A	15	ASP	HA	4.704	0.009	1
1	A	15	ASP	HB2	2.561	0.015	2
1	A	15	ASP	HB3	2.724	0.012	2
1	A	15	ASP	CA	51.697	0.049	1
1	A	15	ASP	CB	42.344	0.075	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	15	ASP	N	117.86	0.028	1
1	A	16	PRO	HA	3.556	0.011	1
1	A	16	PRO	HB2	1.864	0.009	1
1	A	16	PRO	HB3	1.864	0.009	1
1	A	16	PRO	HD2	3.032	0.014	2
1	A	16	PRO	HD3	3.595	0.015	2
1	A	16	PRO	C	178.801	.	1
1	A	16	PRO	CA	64.377	0.038	1
1	A	16	PRO	CB	31.568	0.07	1
1	A	16	PRO	CD	49.9	0.0	1
1	A	16	PRO	CG	26.727	.	1
1	A	17	THR	H	7.858	0.007	1
1	A	17	THR	HA	3.759	0.015	1
1	A	17	THR	HB	4.031	0.009	1
1	A	17	THR	HG21	1.038	0.013	1
1	A	17	THR	HG22	1.038	0.013	1
1	A	17	THR	HG23	1.038	0.013	1
1	A	17	THR	C	176.424	.	1
1	A	17	THR	CA	66.554	0.065	1
1	A	17	THR	CB	67.664	0.057	1
1	A	17	THR	CG2	21.805	0.071	1
1	A	17	THR	N	117.621	0.047	1
1	A	18	SER	H	8.654	0.006	1
1	A	18	SER	HA	3.871	0.008	1
1	A	18	SER	HB2	3.799	0.013	1
1	A	18	SER	HB3	3.799	0.013	1
1	A	18	SER	C	177.038	.	1
1	A	18	SER	CA	61.906	0.051	1
1	A	18	SER	CB	61.877	0.016	1
1	A	18	SER	N	119.883	0.026	1
1	A	19	LYS	H	6.76	0.009	1
1	A	19	LYS	HA	2.613	0.007	1
1	A	19	LYS	HB2	1.396	0.014	2
1	A	19	LYS	HB3	1.593	0.014	2
1	A	19	LYS	HE2	2.793	0.012	1
1	A	19	LYS	HE3	2.793	0.012	1
1	A	19	LYS	HG2	0.997	0.008	1
1	A	19	LYS	HG3	0.997	0.008	1
1	A	19	LYS	C	176.639	.	1
1	A	19	LYS	CA	59.487	0.059	1
1	A	19	LYS	CB	31.586	0.011	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	19	LYS	CD	28.802	.	1
1	A	19	LYS	CE	43.094	.	1
1	A	19	LYS	CG	25.3	0.002	1
1	A	19	LYS	N	121.563	0.025	1
1	A	20	MET	H	7.831	0.01	1
1	A	20	MET	HA	3.927	0.012	1
1	A	20	MET	HB2	2.527	0.014	2
1	A	20	MET	HB3	2.496	0.014	2
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	HG2	2.049	0.013	1
1	A	20	MET	HG3	2.049	0.013	1
1	A	20	MET	C	178.91	.	1
1	A	20	MET	CA	58.719	0.028	1
1	A	20	MET	CB	31.756	0.074	1
1	A	20	MET	CE	16.78	0.058	1
1	A	20	MET	CG	31.692	0.036	1
1	A	20	MET	N	118.908	0.012	1
1	A	21	ARG	H	8.066	0.01	1
1	A	21	ARG	HA	3.905	0.008	1
1	A	21	ARG	HB2	1.648	0.015	1
1	A	21	ARG	HB3	1.648	0.015	1
1	A	21	ARG	HD2	2.995	0.015	1
1	A	21	ARG	HD3	2.995	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	21	ARG	C	179.107	.	1
1	A	21	ARG	CA	58.807	0.029	1
1	A	21	ARG	CB	30.101	0.061	1
1	A	21	ARG	CD	43.078	.	1
1	A	21	ARG	CG	27.802	0.004	1
1	A	21	ARG	N	118.164	0.029	1
1	A	22	HIS	H	7.374	0.008	1
1	A	22	HIS	HA	4.167	0.01	1
1	A	22	HIS	HB2	2.715	0.011	2
1	A	22	HIS	HB3	2.858	0.011	2
1	A	22	HIS	HD2	6.966	0.004	1
1	A	22	HIS	C	178.014	.	1
1	A	22	HIS	CA	58.912	0.066	1
1	A	22	HIS	CB	27.921	0.078	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	22	HIS	CD2	130.823	0.0	1
1	A	22	HIS	N	117.794	0.023	1
1	A	23	LEU	H	8.385	0.01	1
1	A	23	LEU	HA	3.784	0.013	1
1	A	23	LEU	HB2	1.598	0.014	2
1	A	23	LEU	HB3	1.912	0.012	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	23	LEU	C	179.021	.	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	CD1	24.716	0.047	2
1	A	23	LEU	CD2	25.93	0.044	2
1	A	23	LEU	N	122.319	0.052	1
1	A	24	GLU	H	7.122	0.012	1
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	HG2	2.2	0.014	2
1	A	24	GLU	HG3	2.4	0.011	2
1	A	24	GLU	C	178.251	.	1
1	A	24	GLU	CA	58.329	0.058	1
1	A	24	GLU	CB	29.417	0.073	1
1	A	24	GLU	CG	36.091	0.055	1
1	A	24	GLU	N	116.297	0.04	1
1	A	25	THR	H	7.557	0.01	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	25	THR	C	175.17	.	1
1	A	25	THR	CA	63.499	0.059	1
1	A	25	THR	CB	69.177	0.074	1
1	A	25	THR	CG2	21.666	0.065	1
1	A	25	THR	N	108.89	0.04	1
1	A	32	HIS	H	7.072	0.013	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	32	HIS	HA	4.467	.	1
1	A	32	HIS	HB2	2.48	0.006	2
1	A	32	HIS	HB3	2.656	0.012	2
1	A	32	HIS	HD2	6.443	0.006	1
1	A	32	HIS	HE1	7.922	0.006	1
1	A	32	HIS	CA	55.261	.	1
1	A	32	HIS	CB	28.642	0.039	1
1	A	32	HIS	CD2	130.448	0.078	1
1	A	32	HIS	CE1	142.848	0.001	1
1	A	32	HIS	N	118.044	0.05	1
1	A	33	LYS	HB2	1.624	.	1
1	A	33	LYS	HB3	1.624	.	1
1	A	33	LYS	HD2	1.379	.	1
1	A	33	LYS	HD3	1.379	.	1
1	A	33	LYS	HE2	2.805	.	1
1	A	33	LYS	HE3	2.805	.	1
1	A	33	LYS	HG2	1.118	.	1
1	A	33	LYS	HG3	1.118	.	1
1	A	33	LYS	C	175.338	.	1
1	A	33	LYS	CA	55.275	.	1
1	A	33	LYS	CB	34.112	.	1
1	A	33	LYS	CD	28.65	.	1
1	A	33	LYS	CE	41.702	.	1
1	A	33	LYS	CG	24.468	.	1
1	A	34	CYS	H	8.821	0.011	1
1	A	34	CYS	HB2	2.705	.	2
1	A	34	CYS	HB3	3.313	.	2
1	A	34	CYS	CA	57.333	.	1
1	A	34	CYS	CB	30.249	.	1
1	A	34	CYS	N	128.949	0.043	1
1	A	35	PRO	HA	4.338	.	1
1	A	35	PRO	HB2	2.415	.	1
1	A	35	PRO	HB3	2.415	.	1
1	A	35	PRO	HG2	2.017	0.009	1
1	A	35	PRO	HG3	2.017	0.009	1
1	A	35	PRO	C	176.839	.	1
1	A	35	PRO	CA	63.542	0.035	1
1	A	35	PRO	CB	31.808	0.02	1
1	A	35	PRO	CD	50.726	.	1
1	A	35	PRO	CG	26.094	.	1
1	A	36	HIS	H	9.104	0.007	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	36	HIS	CA	55.905	.	1
1	A	36	HIS	CB	29.729	.	1
1	A	36	HIS	N	118.804	0.039	1
1	A	37	CYS	C	173.009	.	1
1	A	38	ASP	H	7.983	0.005	1
1	A	38	ASP	C	175.924	.	1
1	A	38	ASP	CA	55.54	0.025	1
1	A	38	ASP	CB	40.725	0.06	1
1	A	38	ASP	N	115.754	0.018	1
1	A	39	LYS	H	8.148	0.01	1
1	A	39	LYS	HA	3.822	0.014	1
1	A	39	LYS	HB2	1.28	0.006	1
1	A	39	LYS	HB3	1.28	0.006	1
1	A	39	LYS	HD2	1.31	0.014	1
1	A	39	LYS	HD3	1.31	0.014	1
1	A	39	LYS	HE2	2.812	0.011	2
1	A	39	LYS	HE3	3.085	0.0	2
1	A	39	LYS	HG2	1.029	0.006	1
1	A	39	LYS	HG3	1.029	0.006	1
1	A	39	LYS	C	174.515	.	1
1	A	39	LYS	CA	57.889	0.053	1
1	A	39	LYS	CB	33.464	0.051	1
1	A	39	LYS	CD	28.7	0.0	1
1	A	39	LYS	CE	42.555	.	1
1	A	39	LYS	CG	26.009	0.02	1
1	A	39	LYS	N	122.198	0.057	1
1	A	40	LYS	H	7.597	0.006	1
1	A	40	LYS	C	175.043	.	1
1	A	40	LYS	CA	54.586	0.073	1
1	A	40	LYS	CB	35.293	0.046	1
1	A	40	LYS	CD	29.274	.	1
1	A	40	LYS	CG	24.785	.	1
1	A	40	LYS	N	118.804	0.053	1
1	A	41	PHE	H	8.395	0.011	1
1	A	41	PHE	HD1	7.095	0.006	3
1	A	41	PHE	HD2	7.095	0.006	3
1	A	41	PHE	HE1	6.713	0.005	3
1	A	41	PHE	HE2	6.713	0.005	3
1	A	41	PHE	HZ	6.14	0.006	1
1	A	41	PHE	CA	57.208	.	1
1	A	41	PHE	CB	43.475	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	41	PHE	CD1	135.112	.	3
1	A	41	PHE	CD2	135.112	.	3
1	A	41	PHE	CE1	133.781	0.005	3
1	A	41	PHE	CE2	133.781	0.005	3
1	A	41	PHE	CZ	131.989	0.056	1
1	A	41	PHE	N	117.05	0.044	1
1	A	42	ASN	HA	4.19	0.002	1
1	A	42	ASN	HB2	2.12	0.01	1
1	A	42	ASN	HB3	2.12	0.01	1
1	A	42	ASN	C	174.947	.	1
1	A	42	ASN	CA	55.807	0.01	1
1	A	42	ASN	CB	42.016	.	1
1	A	43	GLN	H	7.74	0.013	1
1	A	43	GLN	HG2	2.304	.	1
1	A	43	GLN	HG3	2.304	.	1
1	A	43	GLN	CA	58.492	.	1
1	A	43	GLN	CB	30.33	.	1
1	A	43	GLN	N	118.321	0.06	1
1	A	44	VAL	H	8.859	.	1
1	A	44	VAL	HG11	0.6	0.012	1
1	A	44	VAL	HG12	0.6	0.012	1
1	A	44	VAL	HG13	0.6	0.012	1
1	A	44	VAL	HG21	0.6	0.012	1
1	A	44	VAL	HG22	0.6	0.012	1
1	A	44	VAL	HG23	0.6	0.012	1
1	A	44	VAL	C	177.34	.	1
1	A	44	VAL	CA	65.759	.	1
1	A	44	VAL	CB	31.018	.	1
1	A	44	VAL	N	125.715	.	1
1	A	45	GLY	H	8.87	0.01	1
1	A	45	GLY	HA2	3.563	0.006	2
1	A	45	GLY	HA3	3.765	0.014	2
1	A	45	GLY	C	176.706	.	1
1	A	45	GLY	CA	46.901	0.019	1
1	A	45	GLY	N	108.836	0.06	1
1	A	46	ASN	H	6.995	0.006	1
1	A	46	ASN	HA	4.441	0.015	1
1	A	46	ASN	HB2	2.816	0.013	1
1	A	46	ASN	HB3	2.816	0.013	1
1	A	46	ASN	C	177.372	.	1
1	A	46	ASN	CA	54.836	0.064	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	46	ASN	CB	37.777	0.041	1
1	A	46	ASN	N	118.342	0.044	1
1	A	47	LEU	H	6.876	0.012	1
1	A	47	LEU	HA	2.937	0.011	1
1	A	47	LEU	HB2	1.866	0.015	2
1	A	47	LEU	HB3	1.071	0.013	2
1	A	47	LEU	HD11	0.822	0.013	1
1	A	47	LEU	HD12	0.822	0.013	1
1	A	47	LEU	HD13	0.822	0.013	1
1	A	47	LEU	HD21	0.822	0.013	1
1	A	47	LEU	HD22	0.822	0.013	1
1	A	47	LEU	HD23	0.822	0.013	1
1	A	47	LEU	HG	1.315	0.014	1
1	A	47	LEU	C	177.264	.	1
1	A	47	LEU	CA	57.847	0.039	1
1	A	47	LEU	CB	39.999	0.032	1
1	A	47	LEU	CD1	23.478	.	1
1	A	47	LEU	CD2	23.478	.	1
1	A	47	LEU	CG	26.208	.	1
1	A	47	LEU	N	123.407	0.057	1
1	A	48	LYS	H	8.18	0.009	1
1	A	48	LYS	HA	3.665	0.011	1
1	A	48	LYS	HB2	1.68	0.009	1
1	A	48	LYS	HB3	1.68	0.009	1
1	A	48	LYS	HD2	1.458	0.01	1
1	A	48	LYS	HD3	1.458	0.01	1
1	A	48	LYS	HE2	2.733	0.004	1
1	A	48	LYS	HE3	2.733	0.004	1
1	A	48	LYS	HG2	1.226	0.003	1
1	A	48	LYS	HG3	1.226	0.003	1
1	A	48	LYS	C	178.767	.	1
1	A	48	LYS	CA	59.956	0.018	1
1	A	48	LYS	CB	31.843	0.059	1
1	A	48	LYS	CD	29.097	0.009	1
1	A	48	LYS	CE	42.424	0.042	1
1	A	48	LYS	CG	25.703	0.008	1
1	A	48	LYS	N	117.891	0.044	1
1	A	49	ALA	H	7.193	0.011	1
1	A	49	ALA	HA	3.946	0.011	1
1	A	49	ALA	HB1	1.304	0.013	1
1	A	49	ALA	HB2	1.304	0.013	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	49	ALA	HB3	1.304	0.013	1
1	A	49	ALA	C	179.732	.	1
1	A	49	ALA	CA	54.564	0.067	1
1	A	49	ALA	CB	18.174	0.051	1
1	A	49	ALA	N	119.002	0.03	1
1	A	50	HIS	H	7.324	0.009	1
1	A	50	HIS	HA	4.083	0.015	1
1	A	50	HIS	HB2	3.055	0.014	2
1	A	50	HIS	HB3	2.825	0.012	2
1	A	50	HIS	HD2	7.07	0.007	1
1	A	50	HIS	HE1	7.865	0.015	1
1	A	50	HIS	C	176.003	.	1
1	A	50	HIS	CA	58.898	0.017	1
1	A	50	HIS	CB	28.544	0.069	1
1	A	50	HIS	CD2	130.56	0.037	1
1	A	50	HIS	N	118.664	0.045	1
1	A	51	LEU	H	8.085	0.007	1
1	A	51	LEU	HA	3.676	0.015	1
1	A	51	LEU	HB2	1.803	0.014	2
1	A	51	LEU	HB3	1.486	0.011	2
1	A	51	LEU	HD11	0.886	0.012	1
1	A	51	LEU	HD12	0.886	0.012	1
1	A	51	LEU	HD13	0.886	0.012	1
1	A	51	LEU	HD21	0.886	0.012	1
1	A	51	LEU	HD22	0.886	0.012	1
1	A	51	LEU	HD23	0.886	0.012	1
1	A	51	LEU	HG	1.137	0.004	1
1	A	51	LEU	C	178.47	.	1
1	A	51	LEU	CA	58.047	0.012	1
1	A	51	LEU	CB	41.905	0.044	1
1	A	51	LEU	CD1	25.642	0.076	1
1	A	51	LEU	CD2	25.642	0.076	1
1	A	51	LEU	CG	24.504	0.013	1
1	A	51	LEU	N	116.715	0.006	1
1	A	52	LYS	H	6.883	0.012	1
1	A	52	LYS	HA	3.832	0.011	1
1	A	52	LYS	HB2	1.689	0.009	1
1	A	52	LYS	HB3	1.689	0.009	1
1	A	52	LYS	HD2	1.553	0.013	1
1	A	52	LYS	HD3	1.553	0.013	1
1	A	52	LYS	HE2	2.849	0.002	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	52	LYS	HE3	2.849	0.002	1
1	A	52	LYS	HG2	1.328	0.014	1
1	A	52	LYS	HG3	1.328	0.014	1
1	A	52	LYS	C	178.357	.	1
1	A	52	LYS	CA	58.417	0.034	1
1	A	52	LYS	CB	32.112	0.025	1
1	A	52	LYS	CD	28.897	0.007	1
1	A	52	LYS	CE	40.271	.	1
1	A	52	LYS	CG	24.602	0.005	1
1	A	52	LYS	N	115.588	0.055	1
1	A	53	ILE	H	7.655	0.011	1
1	A	53	ILE	HA	3.831	0.009	1
1	A	53	ILE	HB	1.568	0.013	1
1	A	53	ILE	HG12	0.791	0.011	1
1	A	53	ILE	HG13	0.791	0.011	1
1	A	53	ILE	HG21	0.484	0.014	1
1	A	53	ILE	HG22	0.484	0.014	1
1	A	53	ILE	HG23	0.484	0.014	1
1	A	53	ILE	C	177.054	.	1
1	A	53	ILE	CA	62.683	0.06	1
1	A	53	ILE	CB	37.501	0.044	1
1	A	53	ILE	CD1	14.169	.	1
1	A	53	ILE	CG1	25.093	0.017	1
1	A	53	ILE	CG2	16.399	.	1
1	A	53	ILE	N	115.446	0.037	1
1	A	54	HIS	H	7.1	0.013	1
1	A	54	HIS	HA	4.462	0.004	1
1	A	54	HIS	HB2	2.677	0.013	1
1	A	54	HIS	HB3	2.677	0.013	1
1	A	54	HIS	HD2	6.454	0.002	1
1	A	54	HIS	C	174.896	.	1
1	A	54	HIS	CA	55.395	0.054	1
1	A	54	HIS	CB	28.564	0.065	1
1	A	54	HIS	CD2	130.631	0.005	1
1	A	54	HIS	N	117.283	0.056	1
1	A	55	ILE	H	7.247	0.012	1
1	A	55	ILE	HA	3.884	0.015	1
1	A	55	ILE	HB	1.719	0.01	1
1	A	55	ILE	HD11	0.708	0.012	1
1	A	55	ILE	HD12	0.708	0.012	1
1	A	55	ILE	HD13	0.708	0.012	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	55	ILE	HG12	1.341	0.013	2
1	A	55	ILE	HG13	1.021	0.011	2
1	A	55	ILE	HG21	0.759	0.013	1
1	A	55	ILE	HG22	0.759	0.013	1
1	A	55	ILE	HG23	0.759	0.013	1
1	A	55	ILE	C	175.788	.	1
1	A	55	ILE	CA	61.915	0.073	1
1	A	55	ILE	CB	38.42	0.068	1
1	A	55	ILE	CD1	12.996	0.057	1
1	A	55	ILE	CG1	27.339	0.034	1
1	A	55	ILE	CG2	17.415	0.074	1
1	A	55	ILE	N	119.709	0.047	1
1	A	56	ALA	H	8.009	0.011	1
1	A	56	ALA	HA	4.197	0.014	1
1	A	56	ALA	HB1	1.223	0.013	1
1	A	56	ALA	HB2	1.223	0.013	1
1	A	56	ALA	HB3	1.223	0.013	1
1	A	56	ALA	C	177.042	.	1
1	A	56	ALA	CA	52.204	0.056	1
1	A	56	ALA	CB	19.19	0.068	1
1	A	56	ALA	N	126.276	0.056	1
1	A	57	ASP	H	7.924	0.009	1
1	A	57	ASP	HA	4.447	0.008	1
1	A	57	ASP	HB2	2.516	0.013	1
1	A	57	ASP	HB3	2.516	0.013	1
1	A	57	ASP	C	176.2	.	1
1	A	57	ASP	CA	54.257	0.059	1
1	A	57	ASP	CB	41.256	0.041	1
1	A	57	ASP	N	119.736	0.044	1
1	A	87	PRO	HA	4.165	0.011	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	HD2	3.451	0.009	1
1	A	87	PRO	HD3	3.451	0.009	1
1	A	87	PRO	HG2	1.677	0.007	1
1	A	87	PRO	HG3	1.677	0.007	1
1	A	87	PRO	C	176.103	.	1
1	A	87	PRO	CA	63.071	0.068	1
1	A	87	PRO	CB	31.922	0.036	1
1	A	87	PRO	CD	49.706	0.016	1
1	A	87	PRO	CG	26.478	0.076	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	88	TYR	H	7.917	0.006	1
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	88	TYR	HD1	6.883	0.01	3
1	A	88	TYR	HD2	6.883	0.01	3
1	A	88	TYR	C	174.419	.	1
1	A	88	TYR	CA	57.597	0.042	1
1	A	88	TYR	CB	37.762	0.058	1
1	A	88	TYR	CD1	136.067	0.026	3
1	A	88	TYR	CD2	136.067	0.026	3
1	A	88	TYR	N	119.446	0.054	1
1	A	89	VAL	H	8.195	0.007	1
1	A	89	VAL	HA	4.578	0.011	1
1	A	89	VAL	HB	1.702	0.013	1
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	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	C	175.019	.	1
1	A	89	VAL	CA	60.879	0.054	1
1	A	89	VAL	CB	34.764	0.029	1
1	A	89	VAL	CG1	21.513	0.065	2
1	A	89	VAL	CG2	20.584	0.048	2
1	A	89	VAL	N	123.957	0.037	1
1	A	90	CYS	H	8.869	0.009	1
1	A	90	CYS	HA	4.504	0.013	1
1	A	90	CYS	HB2	2.753	0.012	2
1	A	90	CYS	HB3	3.275	0.01	2
1	A	90	CYS	C	177.11	.	1
1	A	90	CYS	CA	59.226	0.065	1
1	A	90	CYS	CB	29.983	0.071	1
1	A	90	CYS	N	128.789	0.03	1
1	A	91	ILE	H	8.687	0.007	1
1	A	91	ILE	HA	3.915	0.01	1
1	A	91	ILE	HB	1.7	0.007	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

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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	91	ILE	C	175.617	.	1
1	A	91	ILE	CA	62.872	0.064	1
1	A	91	ILE	CB	37.599	0.048	1
1	A	91	ILE	CD1	13.948	.	1
1	A	91	ILE	CG1	28.529	.	1
1	A	91	ILE	CG2	17.542	0.027	1
1	A	91	ILE	N	128.33	0.035	1
1	A	92	HIS	H	8.526	0.015	1
1	A	92	HIS	HA	4.204	0.013	1
1	A	92	HIS	HB2	1.768	0.013	2
1	A	92	HIS	HB3	2.205	0.013	2
1	A	92	HIS	C	176.698	.	1
1	A	92	HIS	CA	57.915	0.038	1
1	A	92	HIS	CB	29.583	0.068	1
1	A	92	HIS	N	121.59	0.059	1
1	A	93	CYS	H	7.958	0.013	1
1	A	93	CYS	HA	5.023	0.007	1
1	A	93	CYS	HB2	3.312	0.015	2
1	A	93	CYS	HB3	2.723	0.014	2
1	A	93	CYS	C	174.973	.	1
1	A	93	CYS	CA	58.432	0.033	1
1	A	93	CYS	CB	32.158	0.072	1
1	A	93	CYS	N	115.876	0.021	1
1	A	94	GLN	H	8.178	0.011	1
1	A	94	GLN	HA	3.876	0.012	1
1	A	94	GLN	HB2	2.306	0.011	2
1	A	94	GLN	HB3	2.186	0.007	2
1	A	94	GLN	HE21	7.129	0.01	1
1	A	94	GLN	HE22	6.368	0.004	1
1	A	94	GLN	HG2	2.099	0.015	1
1	A	94	GLN	HG3	2.099	0.015	1
1	A	94	GLN	C	174.707	.	1
1	A	94	GLN	CA	58.288	0.073	1
1	A	94	GLN	CB	25.429	0.055	1
1	A	94	GLN	CG	34.36	0.054	1
1	A	94	GLN	N	116.348	0.034	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	94	GLN	NE2	112.157	0.053	1
1	A	95	ARG	H	7.856	0.011	1
1	A	95	ARG	HA	3.927	0.012	1
1	A	95	ARG	HB2	1.354	0.012	2
1	A	95	ARG	HB3	1.201	0.015	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	HG2	1.705	0.011	2
1	A	95	ARG	HG3	1.671	0.015	2
1	A	95	ARG	C	174.113	.	1
1	A	95	ARG	CA	57.979	0.031	1
1	A	95	ARG	CB	31.403	0.038	1
1	A	95	ARG	CD	43.547	0.078	1
1	A	95	ARG	CG	28.398	0.018	1
1	A	95	ARG	N	121.105	0.053	1
1	A	96	GLN	H	7.833	0.007	1
1	A	96	GLN	HA	4.845	0.011	1
1	A	96	GLN	HB2	2.034	0.014	1
1	A	96	GLN	HB3	2.034	0.014	1
1	A	96	GLN	HG2	2.189	0.012	1
1	A	96	GLN	HG3	2.189	0.012	1
1	A	96	GLN	C	174.982	.	1
1	A	96	GLN	CA	54.273	0.056	1
1	A	96	GLN	CB	31.188	0.035	1
1	A	96	GLN	CG	34.06	.	1
1	A	96	GLN	N	119.07	0.045	1
1	A	97	PHE	H	8.875	0.008	1
1	A	97	PHE	HA	4.456	0.014	1
1	A	97	PHE	HB2	2.596	0.009	2
1	A	97	PHE	HB3	3.114	0.011	2
1	A	97	PHE	HD1	7.039	0.012	3
1	A	97	PHE	HD2	7.039	0.012	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	HZ	5.869	0.005	1
1	A	97	PHE	C	174.888	.	1
1	A	97	PHE	CA	57.285	0.011	1
1	A	97	PHE	CB	43.463	0.069	1
1	A	97	PHE	CD1	135.172	0.041	3
1	A	97	PHE	CD2	135.172	0.041	3
1	A	97	PHE	CZ	131.433	0.017	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	97	PHE	N	118.706	0.052	1
1	A	98	ALA	H	9.019	0.01	1
1	A	98	ALA	HA	4.462	0.014	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	C	176.342	.	1
1	A	98	ALA	CA	53.297	0.015	1
1	A	98	ALA	CB	19.97	0.057	1
1	A	98	ALA	N	121.599	0.032	1
1	A	99	ASP	H	7.323	0.006	1
1	A	99	ASP	HA	4.742	0.013	1
1	A	99	ASP	HB2	2.535	0.014	2
1	A	99	ASP	HB3	2.666	0.013	2
1	A	99	ASP	CA	51.162	0.064	1
1	A	99	ASP	CB	42.663	0.035	1
1	A	99	ASP	N	114.064	0.051	1
1	A	100	PRO	HA	3.463	0.014	1
1	A	100	PRO	HB2	1.712	0.012	2
1	A	100	PRO	HB3	1.641	0.011	2
1	A	100	PRO	HD2	3.025	0.008	2
1	A	100	PRO	HD3	3.617	0.01	2
1	A	100	PRO	HG2	1.556	0.007	2
1	A	100	PRO	HG3	1.811	0.014	2
1	A	100	PRO	C	178.935	.	1
1	A	100	PRO	CA	64.03	0.075	1
1	A	100	PRO	CB	31.142	0.071	1
1	A	100	PRO	CD	50.016	0.034	1
1	A	100	PRO	CG	26.824	0.024	1
1	A	101	GLY	H	8.262	0.01	1
1	A	101	GLY	HA2	3.63	0.011	1
1	A	101	GLY	HA3	3.63	0.011	1
1	A	101	GLY	C	175.852	.	1
1	A	101	GLY	CA	46.678	0.054	1
1	A	101	GLY	N	110.226	0.057	1
1	A	102	ALA	H	8.019	0.005	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	102	ALA	C	180.54	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	102	ALA	CA	54.496	0.046	1
1	A	102	ALA	CB	18.812	0.071	1
1	A	102	ALA	N	125.555	0.035	1
1	A	103	LEU	H	6.789	0.009	1
1	A	103	LEU	HA	2.975	0.008	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	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	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	HG	1.429	0.01	1
1	A	103	LEU	C	176.809	.	1
1	A	103	LEU	CA	57.588	0.064	1
1	A	103	LEU	CB	40.519	0.066	1
1	A	103	LEU	CD1	23.066	0.038	2
1	A	103	LEU	CD2	23.359	0.026	2
1	A	103	LEU	CG	26.606	.	1
1	A	103	LEU	N	118.329	0.033	1
1	A	104	GLN	H	7.861	0.009	1
1	A	104	GLN	HA	3.8	0.011	1
1	A	104	GLN	HB2	1.99	0.014	1
1	A	104	GLN	HB3	1.99	0.014	1
1	A	104	GLN	HE21	6.657	0.015	1
1	A	104	GLN	HE22	7.476	0.011	1
1	A	104	GLN	HG2	2.22	0.015	2
1	A	104	GLN	HG3	2.304	0.009	2
1	A	104	GLN	C	178.34	.	1
1	A	104	GLN	CA	58.869	0.057	1
1	A	104	GLN	CB	27.988	0.053	1
1	A	104	GLN	CG	33.706	0.078	1
1	A	104	GLN	N	118.337	0.053	1
1	A	104	GLN	NE2	111.002	0.052	1
1	A	105	ARG	H	7.707	0.005	1
1	A	105	ARG	HA	3.815	0.009	1
1	A	105	ARG	HB2	1.64	0.011	1
1	A	105	ARG	HB3	1.639	0.011	1
1	A	105	ARG	HD2	3.062	0.008	1
1	A	105	ARG	HD3	3.062	0.008	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	105	ARG	HG2	1.332	0.008	1
1	A	105	ARG	HG3	1.332	0.008	1
1	A	105	ARG	C	178.351	.	1
1	A	105	ARG	CA	58.968	0.054	1
1	A	105	ARG	CB	30.21	0.055	1
1	A	105	ARG	CD	43.004	0.009	1
1	A	105	ARG	CG	28.003	0.008	1
1	A	105	ARG	N	116.516	0.04	1
1	A	106	HIS	H	7.363	0.01	1
1	A	106	HIS	HA	4.103	0.014	1
1	A	106	HIS	HB2	2.703	0.011	2
1	A	106	HIS	HB3	2.9	0.01	2
1	A	106	HIS	HD2	6.681	0.004	1
1	A	106	HIS	HE1	7.878	.	1
1	A	106	HIS	C	176.619	.	1
1	A	106	HIS	CA	59.059	0.077	1
1	A	106	HIS	CB	28.524	0.075	1
1	A	106	HIS	N	118.237	0.053	1
1	A	107	VAL	H	8.352	0.008	1
1	A	107	VAL	HA	3.473	0.012	1
1	A	107	VAL	HB	2.207	0.014	1
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	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	C	176.81	.	1
1	A	107	VAL	CA	66.042	0.036	1
1	A	107	VAL	CB	31.888	0.07	1
1	A	107	VAL	CG1	22.376	0.024	2
1	A	107	VAL	CG2	21.848	0.048	2
1	A	107	VAL	N	114.907	0.041	1
1	A	108	ARG	H	6.735	0.008	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	108	ARG	HD2	3.048	0.007	1
1	A	108	ARG	HD3	3.048	0.007	1
1	A	108	ARG	HG2	1.515	0.01	1
1	A	108	ARG	HG3	1.515	0.01	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	108	ARG	C	178.341	.	1
1	A	108	ARG	CA	57.871	0.067	1
1	A	108	ARG	CB	29.759	0.041	1
1	A	108	ARG	CD	43.062	0.065	1
1	A	108	ARG	CG	27.003	0.006	1
1	A	108	ARG	N	117.784	0.052	1
1	A	109	ILE	H	7.712	0.01	1
1	A	109	ILE	HA	3.813	0.015	1
1	A	109	ILE	HB	1.548	0.013	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	HG12	0.754	0.015	2
1	A	109	ILE	HG13	0.815	0.015	2
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	C	176.877	.	1
1	A	109	ILE	CA	63.016	0.054	1
1	A	109	ILE	CB	37.442	0.052	1
1	A	109	ILE	CD1	14.638	0.053	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	N	116.281	0.024	1
1	A	110	HIS	H	7.299	0.008	1
1	A	110	HIS	HA	4.476	0.015	1
1	A	110	HIS	HB2	2.6	0.01	2
1	A	110	HIS	HB3	2.481	0.002	2
1	A	110	HIS	HD2	6.574	0.009	1
1	A	110	HIS	HE1	7.913	.	1
1	A	110	HIS	C	175.597	.	1
1	A	110	HIS	CA	55.29	0.016	1
1	A	110	HIS	CB	28.463	0.032	1
1	A	110	HIS	CD2	131.677	0.047	1
1	A	110	HIS	N	117.512	0.029	1
1	A	111	THR	H	7.528	0.012	1
1	A	111	THR	HA	4.135	0.015	1
1	A	111	THR	HB	4.176	0.014	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

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	111	THR	C	174.74	.	1
1	A	111	THR	CA	62.068	0.059	1
1	A	111	THR	CB	69.863	0.068	1
1	A	111	THR	CG2	21.179	0.058	1
1	A	111	THR	N	109.948	0.055	1
1	A	112	GLY	H	7.878	0.009	1
1	A	112	GLY	HA2	3.751	0.011	2
1	A	112	GLY	HA3	3.548	0.014	2
1	A	112	GLY	CA	46.168	0.065	1
1	A	112	GLY	N	117.415	0.04	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	-0.22 ± 0.24	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	95	0.50 ± 0.36	None needed (imprecise)
$^{13}C'$	94	-0.27 ± 0.22	None needed (< 0.5 ppm)
^{15}N	95	0.90 ± 0.71	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 85%, i.e. 297 atoms were assigned a chemical shift out of a possible 348. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	121/122 (99%)	49/50 (98%)	48/48 (100%)	24/24 (100%)
Sidechain	162/202 (80%)	112/129 (87%)	49/59 (83%)	1/14 (7%)
Aromatic	14/24 (58%)	7/13 (54%)	7/9 (78%)	0/2 (0%)
Overall	297/348 (85%)	168/192 (88%)	104/116 (90%)	25/40 (62%)

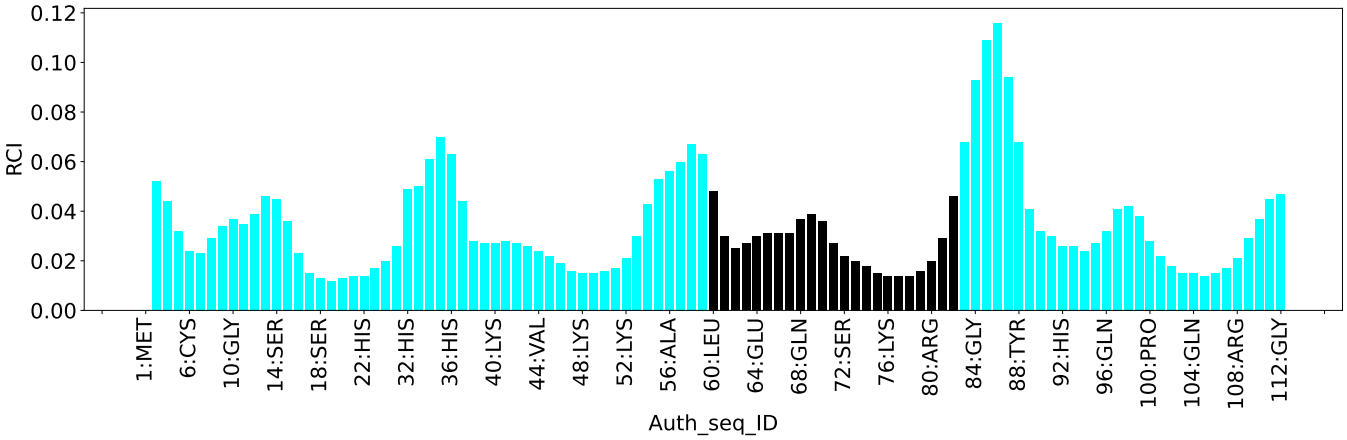
7.1.4 Statistically unusual chemical shifts (i)

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:



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	525
Intra-residue (|i-j|=0)	231
Sequential (|i-j|=1)	123
Medium range (|i-j|>1 and |i-j|<5)	95
Long range (|i-j|≥5)	76
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	53
Number of unmapped restraints	0
Number of restraints per residue	5.1
Number of long range restraints per residue[1]	0.7

[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)	4.8	0.2
0.2-0.5 (Medium)	6.6	0.49
>0.5 (Large)	3.0	1.69

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)	3.9	4.98
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

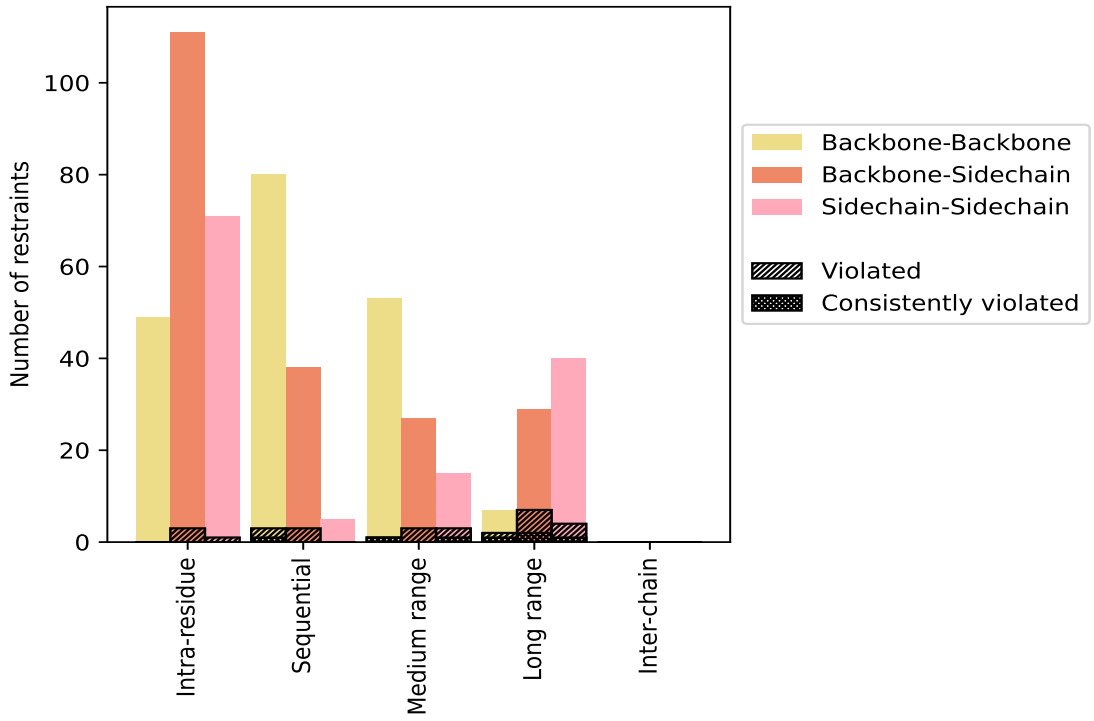
9.1 Summary of distance violations (i)

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)	231	44.0	4	1.7	0.8	0	0.0	0.0
Backbone-Backbone	49	9.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	111	21.1	3	2.7	0.6	0	0.0	0.0
Sidechain-Sidechain	71	13.5	1	1.4	0.2	0	0.0	0.0
Sequential (|i-j|=1)	123	23.4	6	4.9	1.1	1	0.8	0.2
Backbone-Backbone	80	15.2	3	3.8	0.6	1	1.2	0.2
Backbone-Sidechain	38	7.2	3	7.9	0.6	0	0.0	0.0
Sidechain-Sidechain	5	1.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	95	18.1	7	7.4	1.3	2	2.1	0.4
Backbone-Backbone	53	10.1	1	1.9	0.2	1	1.9	0.2
Backbone-Sidechain	27	5.1	3	11.1	0.6	0	0.0	0.0
Sidechain-Sidechain	15	2.9	3	20.0	0.6	1	6.7	0.2
Long range (|i-j|≥5)	76	14.5	13	17.1	2.5	4	5.3	0.8
Backbone-Backbone	7	1.3	2	28.6	0.4	1	14.3	0.2
Backbone-Sidechain	29	5.5	7	24.1	1.3	2	6.9	0.4
Sidechain-Sidechain	40	7.6	4	10.0	0.8	1	2.5	0.2
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	525	100.0	30	5.7	5.7	7	1.3	1.3
Backbone-Backbone	189	36.0	6	3.2	1.1	3	1.6	0.6
Backbone-Sidechain	205	39.0	16	7.8	3.0	2	1.0	0.4
Sidechain-Sidechain	131	25.0	8	6.1	1.5	2	1.5	0.4

[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	3	5	7	0	15	0.31	0.91	0.23	0.28
2	0	3	5	8	0	16	0.4	1.23	0.33	0.27
3	0	2	4	7	0	13	0.41	0.98	0.23	0.31
4	0	4	4	7	0	15	0.42	1.55	0.39	0.24
5	1	2	5	5	0	13	0.28	0.77	0.19	0.23
6	2	3	4	5	0	14	0.31	0.8	0.22	0.22
7	1	2	4	7	0	14	0.31	0.81	0.2	0.26
8	1	3	4	8	0	16	0.34	0.97	0.23	0.29
9	0	4	4	6	0	14	0.41	1.69	0.44	0.22
10	0	3	3	7	0	13	0.29	0.79	0.22	0.21

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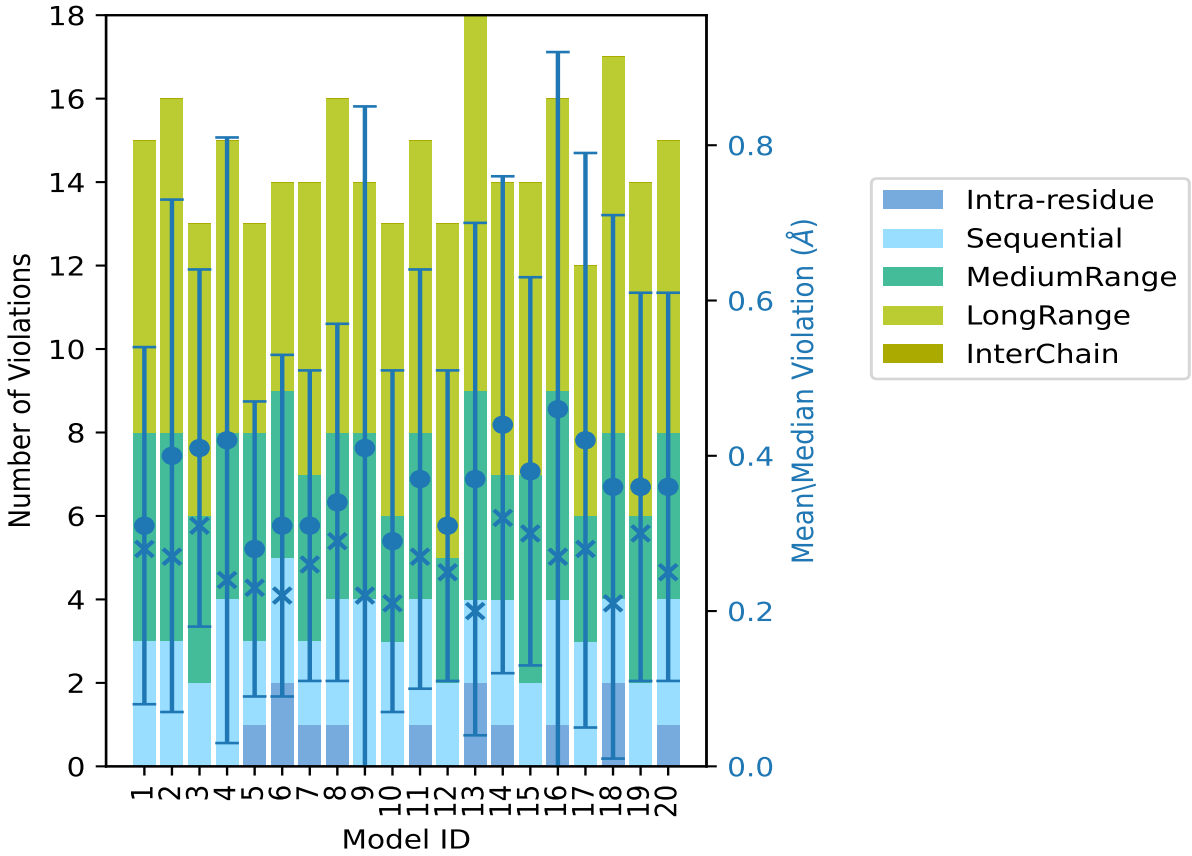
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	1	3	4	7	0	15	0.37	0.96	0.27	0.27
12	0	2	3	8	0	13	0.31	0.87	0.2	0.25
13	2	2	5	9	0	18	0.37	1.34	0.33	0.2
14	1	3	3	7	0	14	0.44	1.32	0.32	0.32
15	0	2	5	7	0	14	0.38	1.04	0.25	0.3
16	1	3	5	7	0	16	0.46	1.54	0.46	0.27
17	0	3	3	6	0	12	0.42	1.4	0.37	0.28
18	2	2	4	9	0	17	0.36	1.39	0.35	0.21
19	0	2	4	8	0	14	0.36	0.89	0.25	0.3
20	1	3	4	7	0	15	0.36	0.88	0.25	0.25

[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

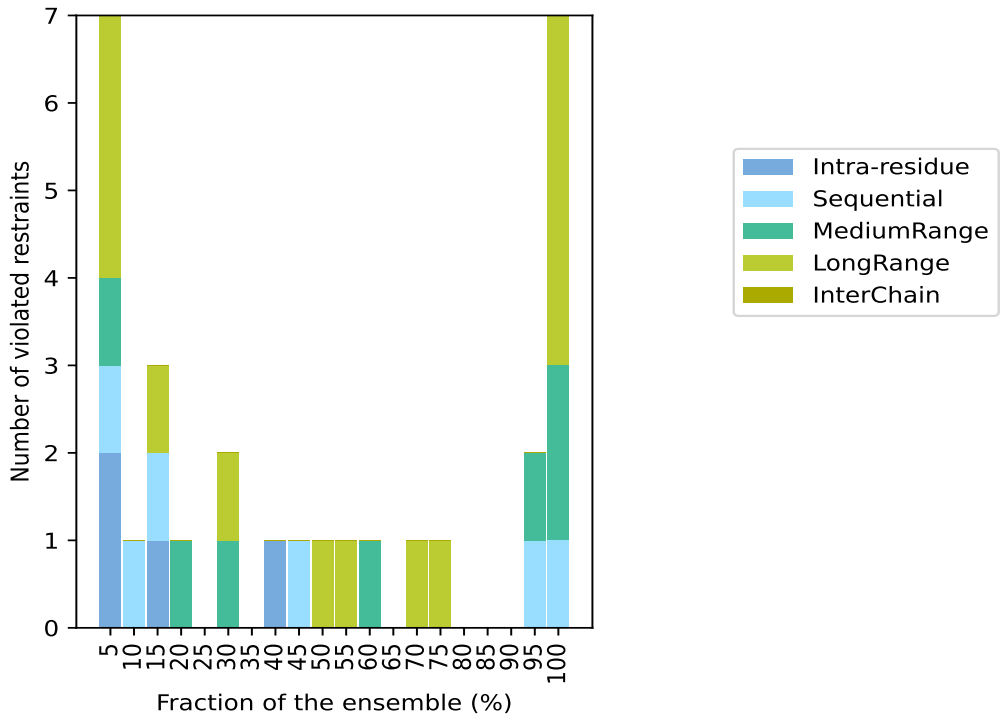
9.3 Distance violation statistics for the ensemble (i)

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, 495(IR:227, SQ:117, MR:88, LR:63, 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]	%
2	1	1	3	0	7	1	5.0
0	1	0	0	0	1	2	10.0
1	1	0	1	0	3	3	15.0
0	0	1	0	0	1	4	20.0
0	0	0	0	0	0	5	25.0
0	0	1	1	0	2	6	30.0
0	0	0	0	0	0	7	35.0
1	0	0	0	0	1	8	40.0
0	1	0	0	0	1	9	45.0
0	0	0	1	0	1	10	50.0
0	0	0	1	0	1	11	55.0
0	0	1	0	0	1	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	1	0	1	14	70.0
0	0	0	1	0	1	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	1	1	0	0	2	19	95.0
0	1	2	4	0	7	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

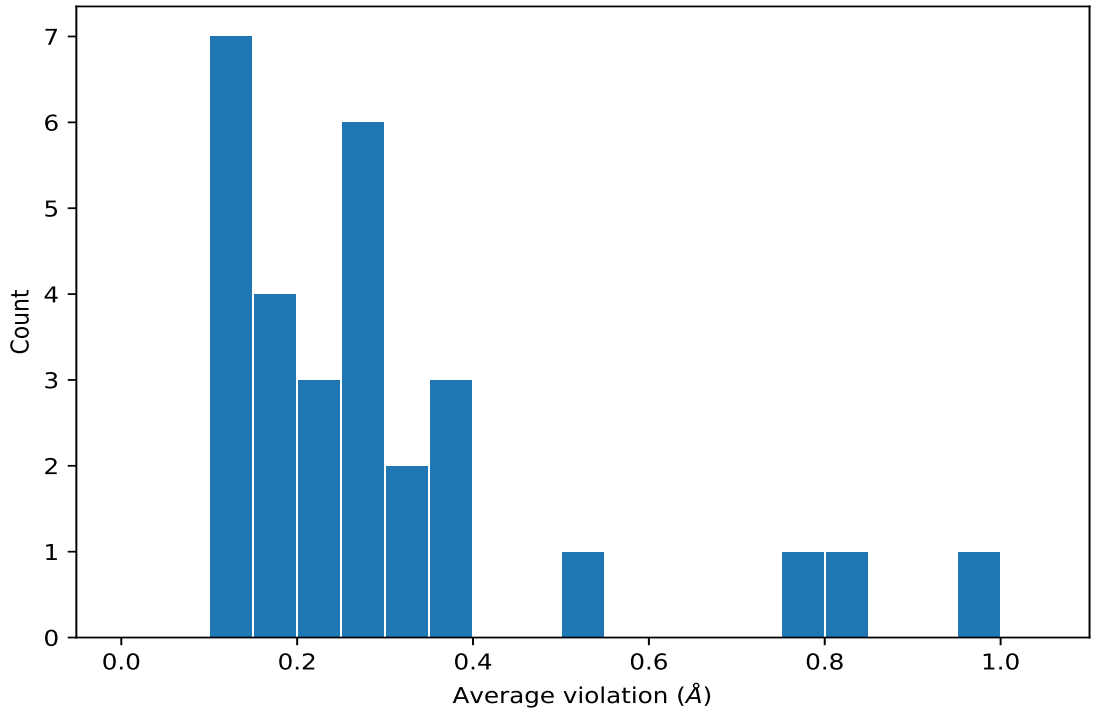
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 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. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

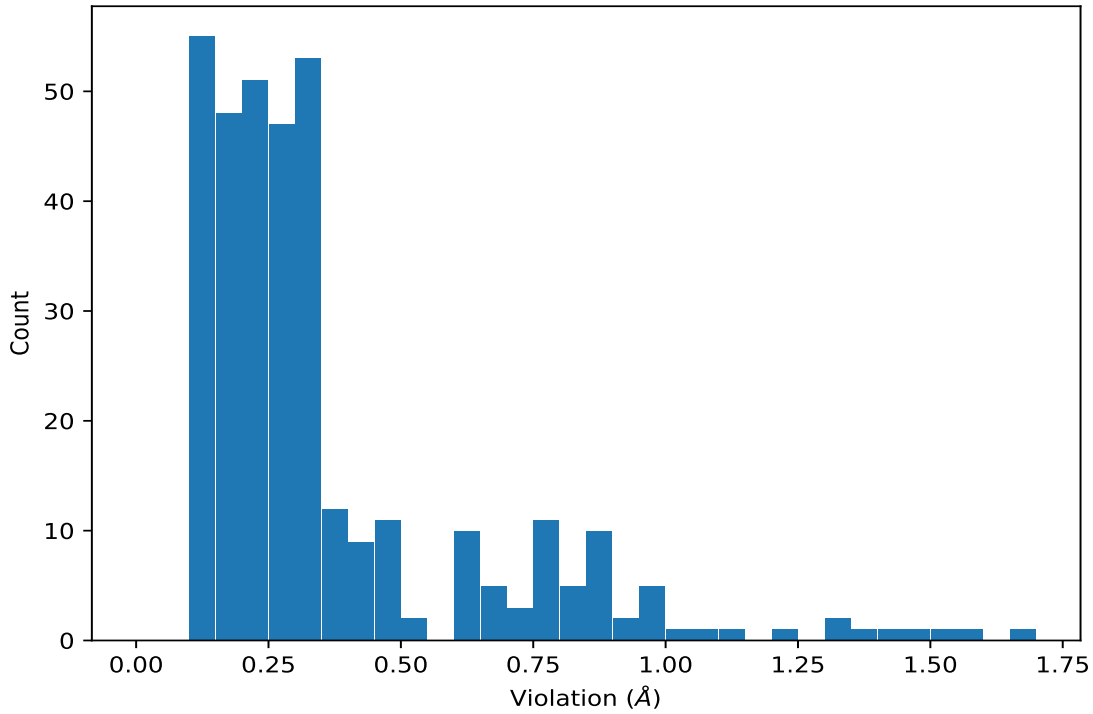
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,92)	1:60:A:LEU:H	1:68:A:GLN:HE22	20	0.99	0.38	0.94
(1,66)	1:79:A:LEU:HG	1:75:A:LEU:HB2	20	0.82	0.08	0.8
(1,346)	1:82:A:HIS:HE1	1:65:A:CYS:HB2	20	0.35	0.13	0.32
(1,232)	1:68:A:GLN:H	1:62:A:CYS:HB3	20	0.3	0.11	0.29
(1,310)	1:69:A:PHE:H	1:60:A:LEU:HA	20	0.26	0.05	0.26
(1,400)	1:60:A:LEU:H	1:58:A:GLY:HA2	20	0.23	0.11	0.19
(1,445)	1:67:A:LYS:H	1:68:A:GLN:H	20	0.22	0.03	0.21
(1,316)	1:80:A:ARG:H	1:79:A:LEU:HB3	19	0.25	0.05	0.28
(1,84)	1:66:A:GLY:H	1:62:A:CYS:HB2	19	0.18	0.04	0.16
(1,12)	1:68:A:GLN:HE22	1:60:A:LEU:H	15	0.54	0.3	0.44

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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)
(1,92)	1:60:A:LEU:H	1:68:A:GLN:HE22	9	1.69
(1,92)	1:60:A:LEU:H	1:68:A:GLN:HE22	4	1.55
(1,258)	1:80:A:ARG:HA	1:85:A:GLU:HB3	16	1.54
(1,92)	1:60:A:LEU:H	1:68:A:GLN:HE22	16	1.49
(1,92)	1:60:A:LEU:H	1:68:A:GLN:HE22	17	1.4
(1,92)	1:60:A:LEU:H	1:68:A:GLN:HE22	18	1.39
(1,258)	1:80:A:ARG:HA	1:85:A:GLU:HB3	13	1.34
(1,92)	1:60:A:LEU:H	1:68:A:GLN:HE22	14	1.32
(1,258)	1:80:A:ARG:HA	1:85:A:GLU:HB3	2	1.23
(1,92)	1:60:A:LEU:H	1:68:A:GLN:HE22	2	1.11

10 Dihedral-angle violation analysis

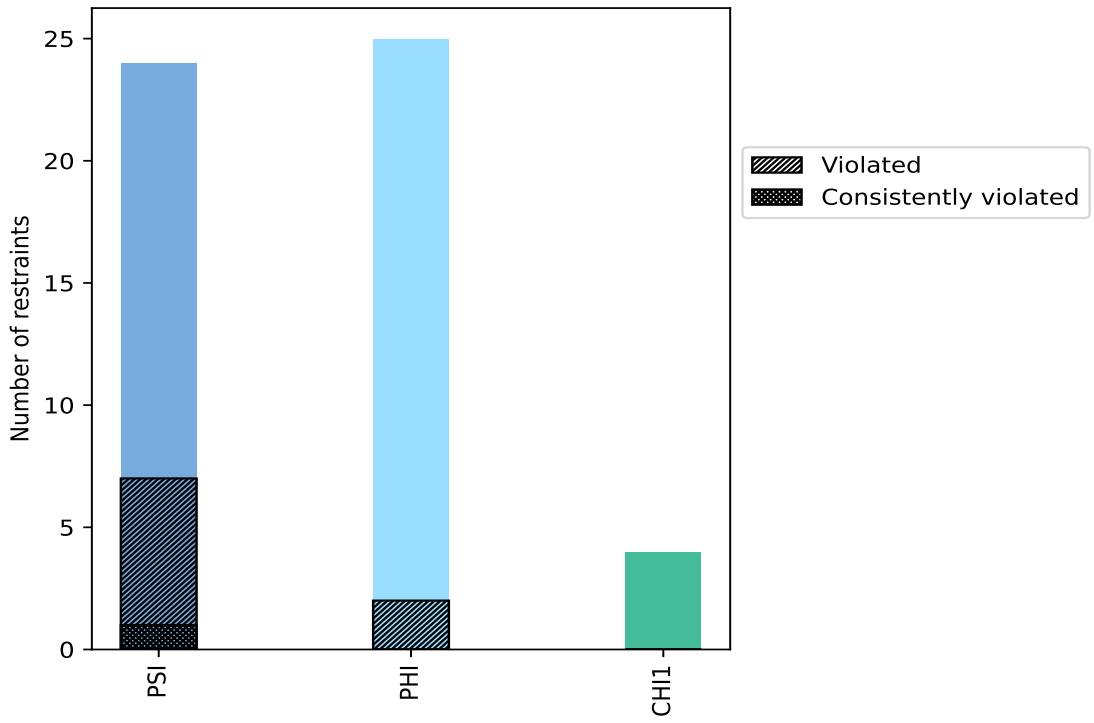
10.1 Summary of dihedral-angle violations

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	24	45.3	7	29.2	13.2	1	4.2	1.9
PHI	25	47.2	2	8.0	3.8	0	0.0	0.0
CHI1	4	7.5	0	0.0	0.0	0	0.0	0.0
Total	53	100.0	9	17.0	17.0	1	1.9	1.9

[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



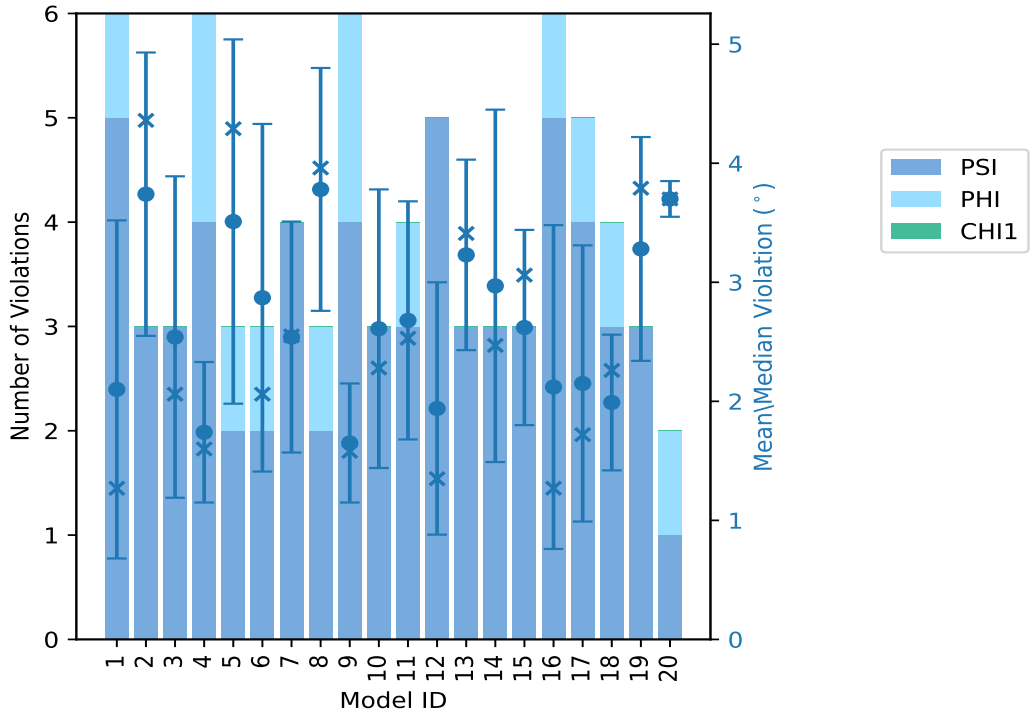
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	5	1	0	6	2.1	4.91	1.42	1.27
2	3	0	0	3	3.74	4.79	1.19	4.36
3	3	0	0	3	2.54	4.39	1.35	2.06
4	4	2	0	6	1.74	2.86	0.59	1.6
5	2	1	0	3	3.51	4.87	1.53	4.29
6	2	1	0	3	2.87	4.92	1.46	2.06
7	4	0	0	4	2.54	3.89	0.97	2.55
8	2	1	0	3	3.78	4.94	1.02	3.96
9	4	2	0	6	1.65	2.27	0.5	1.58
10	3	0	0	3	2.61	4.17	1.17	2.28
11	3	1	0	4	2.68	4.13	1.0	2.53
12	5	0	0	5	1.94	3.88	1.06	1.35
13	3	0	0	3	3.23	4.11	0.8	3.41
14	3	0	0	3	2.97	4.98	1.48	2.47
15	3	0	0	3	2.62	3.33	0.82	3.06
16	5	1	0	6	2.12	4.15	1.36	1.27
17	4	1	0	5	2.15	4.01	1.16	1.72
18	3	1	0	4	1.99	2.41	0.57	2.26
19	3	0	0	3	3.28	4.09	0.94	3.79
20	1	1	0	2	3.7	3.85	0.15	3.7

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble

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]	%
2	0	0	2	1	5.0
0	1	0	1	2	10.0
1	0	0	1	3	15.0
0	0	0	0	4	20.0
0	0	0	0	5	25.0
0	0	0	0	6	30.0
1	0	0	1	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	1	0	1	11	55.0

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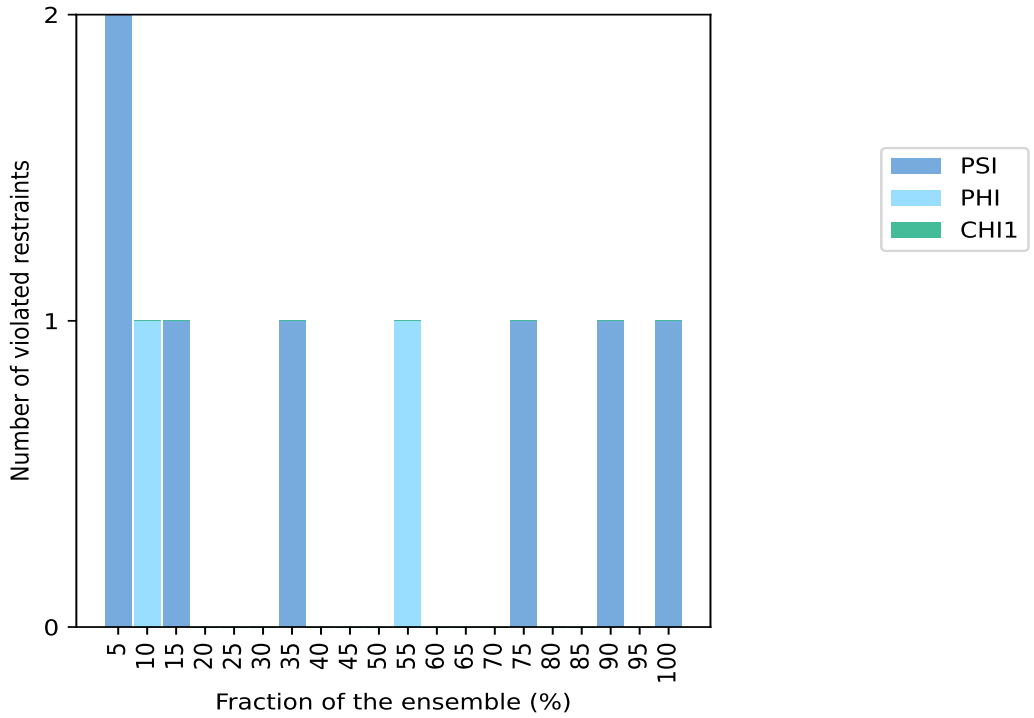
Number of violated restraints				Fraction of the ensemble	
PSI	PHI	CHI1	Total	Count[1]	%
0	0	0	0	12	60.0
0	0	0	0	13	65.0
0	0	0	0	14	70.0
1	0	0	1	15	75.0
0	0	0	0	16	80.0
0	0	0	0	17	85.0
1	0	0	1	18	90.0
0	0	0	0	19	95.0
1	0	0	1	20	100.0

[1] Number of models with violations

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

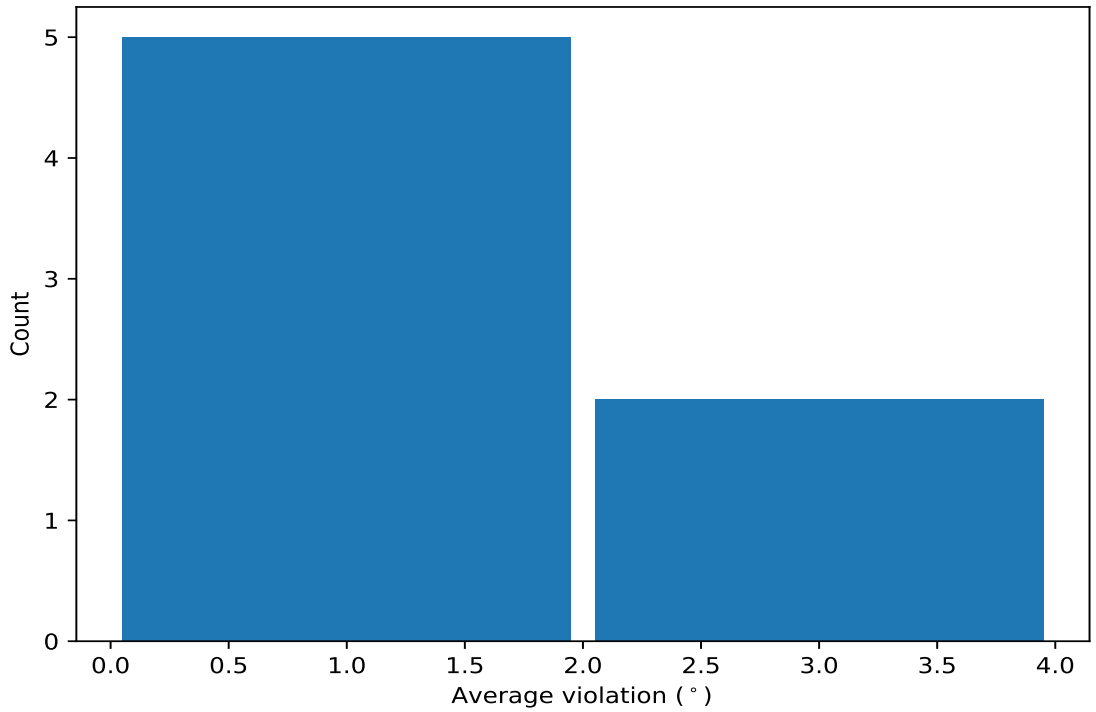


10.4 Most violated dihedral-angle restraints in the ensemble

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 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.

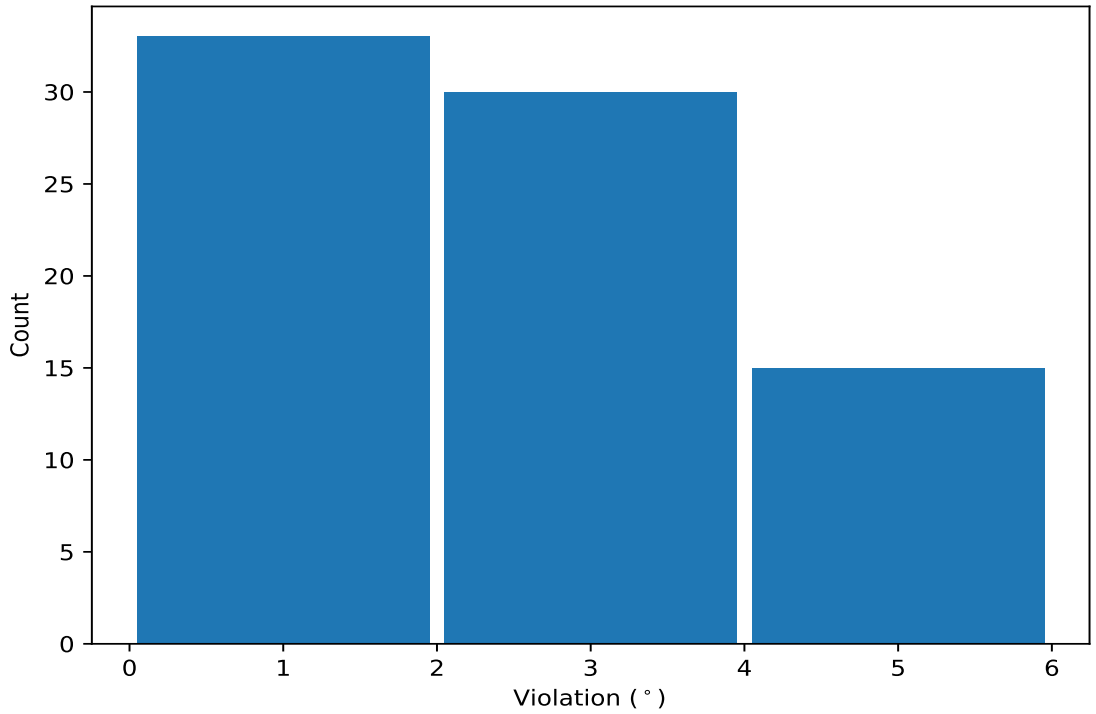
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,6)	1:59:A:PRO:N	1:59:A:PRO:CA	1:59:A:PRO:C	1:60:A:LEU:N	20	3.78	0.94	3.98
(1,20)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:GLN:N	18	3.23	0.95	3.02
(1,16)	1:65:A:CYS:N	1:65:A:CYS:CA	1:65:A:CYS:C	1:66:A:GLY:N	15	1.61	0.43	1.48
(1,7)	1:60:A:LEU:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	11	1.76	0.81	1.44
(1,26)	1:71:A:THR:N	1:71:A:THR:CA	1:71:A:THR:C	1:72:A:SER:N	7	1.47	0.42	1.31
(1,42)	1:79:A:LEU:N	1:79:A:LEU:CA	1:79:A:LEU:C	1:80:A:ARG:N	3	1.07	0.03	1.05
(1,53)	1:85:A:GLU:C	1:86:A:LYS:N	1:86:A:LYS:CA	1:86:A:LYS:C	2	1.48	0.36	1.48

[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 violations for 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 (°)
(1,6)	1:59:A:PRO:N	1:59:A:PRO:CA	1:59:A:PRO:C	1:60:A:LEU:N	14	4.98
(1,20)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:GLN:N	8	4.94
(1,6)	1:59:A:PRO:N	1:59:A:PRO:CA	1:59:A:PRO:C	1:60:A:LEU:N	6	4.92
(1,6)	1:59:A:PRO:N	1:59:A:PRO:CA	1:59:A:PRO:C	1:60:A:LEU:N	1	4.91
(1,6)	1:59:A:PRO:N	1:59:A:PRO:CA	1:59:A:PRO:C	1:60:A:LEU:N	5	4.87
(1,6)	1:59:A:PRO:N	1:59:A:PRO:CA	1:59:A:PRO:C	1:60:A:LEU:N	2	4.79
(1,20)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:GLN:N	3	4.39
(1,20)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:GLN:N	2	4.36
(1,20)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:GLN:N	5	4.29
(1,6)	1:59:A:PRO:N	1:59:A:PRO:CA	1:59:A:PRO:C	1:60:A:LEU:N	10	4.17