



wwPDB NMR Structure Validation Summary Report ⓘ

Dec 25, 2024 – 12:26 AM EST

PDB ID : 2N25
BMRB ID : 25587
Title : Solution structure of Miz-1 zinc finger 2
Authors : Bedard, M.; Lavigne, P.
Deposited on : 2015-04-28

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

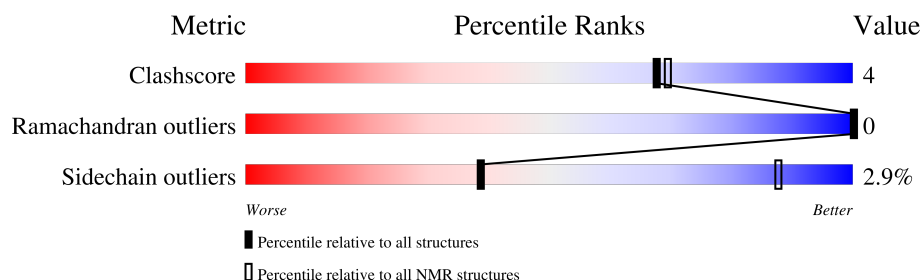
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 74%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	112	

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:32-A:56 (25)	0.52	2

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

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

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

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 441 atoms, of which 218 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
1	A	29	Total	C	H	N	O	S	0
			440	138	218	41	40	3	

There is a discrepancy between the modelled and reference sequences:

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

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

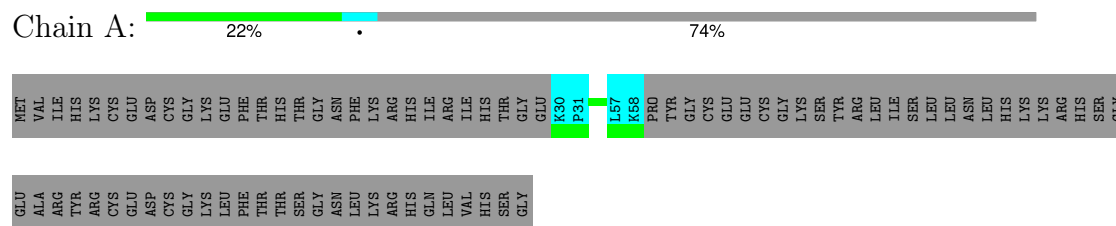
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

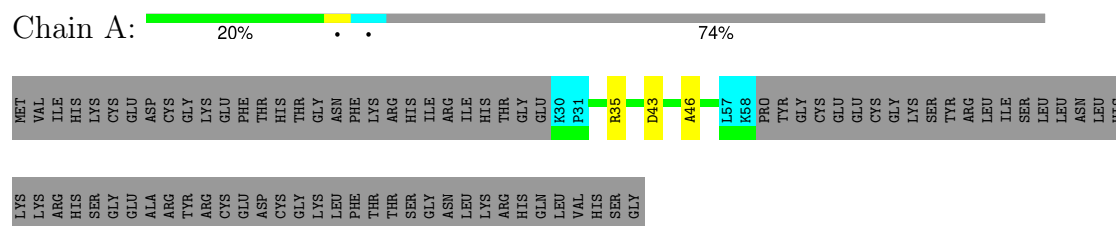
- Molecule 1: Zinc finger and BTB domain-containing protein 17



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

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

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



5 Refinement protocol and experimental data overview

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

Of the 300 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

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

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1018
Number of shifts mapped to atoms	257
Number of unparsed shifts	0
Number of shifts with mapping errors	761
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	74%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	189	174	174	1±1
All	All	3800	3480	3480	26

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 4.

5 of 19 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:GLU:HG2	1:A:37:CYS:SG	0.70	2.25	16	1
1:A:34:CYS:SG	1:A:50:HIS:CD2	0.59	2.95	3	2
1:A:48:LYS:O	1:A:52:LYS:HG2	0.57	2.00	12	1
1:A:36:GLU:HB2	1:A:54:HIS:CE1	0.53	2.39	10	2
1:A:43:ASP:HB3	1:A:46:ALA:CB	0.50	2.36	1	3

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	25/112 (22%)	25±1 (98±3%)	0±1 (2±3%)	0±0 (0±0%)	100	100
All	All	500/2240 (22%)	491 (98%)	9 (2%)	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	21/98 (21%)	20±1 (97±4%)	1±1 (3±4%)	39	88
All	All	420/1960 (21%)	408 (97%)	12 (3%)	39	88

5 of 6 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	36	GLU	5
1	A	34	CYS	3
1	A	35	ARG	1
1	A	42	SER	1
1	A	54	HIS	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 74% for the well-defined parts and 70% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping

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

Total number of shifts	1018
Number of shifts mapped to atoms	257
Number of unparsed shifts	0
Number of shifts with mapping errors	761
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 761) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	74	LEU	N	121.032	0.022	1
1	A	74	LEU	H	6.398	0.005	1
1	A	74	LEU	CA	56.662	0.016	1
1	A	74	LEU	CB	41.474	0.039	1
1	A	77	LEU	N	120.426	0.018	1
1	A	77	LEU	H	7.292	0.007	1
1	A	77	LEU	CB	41.962	0.026	1
1	A	77	LEU	CA	57.821	0.003	1
1	A	76	ASN	N	117.934	0.018	1
1	A	76	ASN	H	8.455	0.008	1
1	A	76	ASN	CA	55.825	0.042	1
1	A	76	ASN	CB	36.938	0.035	1
1	A	75	LEU	H	7.051	0.005	1
1	A	75	LEU	N	122.14	0.028	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	78	HIS	N	119.946	0.025	1
1	A	78	HIS	H	7.448	0.007	1
1	A	78	HIS	CB	27.697	0.07	1
1	A	78	HIS	CA	59.176	0.017	1
1	A	79	LYS	H	8.417	0.006	1
1	A	79	LYS	N	116.51	0.042	1
1	A	79	LYS	CB	32.257	0.042	1
1	A	79	LYS	CA	59.818	0.008	1
1	A	80	LYS	H	7.095	0.004	1
1	A	80	LYS	N	118.121	0.026	1
1	A	80	LYS	CA	58.342	0.013	1
1	A	80	LYS	CB	31.97	0.022	1
1	A	81	ARG	H	7.628	0.007	1
1	A	81	ARG	N	116.756	0.022	1
1	A	81	ARG	CB	29.22	0.025	1
1	A	81	ARG	CA	57.114	0.029	1
1	A	82	HIS	H	7.142	0.008	1
1	A	82	HIS	N	116.234	0.077	1
1	A	82	HIS	CA	55.048	0.013	1
1	A	82	HIS	CB	28.511	0.045	1
1	A	83	SER	N	115.019	0.041	1
1	A	83	SER	H	7.741	0.004	1
1	A	83	SER	CA	58.553	0.026	1
1	A	83	SER	CB	63.562	0.028	1
1	A	85	GLU	H	7.943	0.004	1
1	A	85	GLU	N	120.002	0.065	1
1	A	85	GLU	CA	56.324	0.047	1
1	A	85	GLU	CB	30.421	0.011	1
1	A	84	GLY	H	8.227	0.015	1
1	A	84	GLY	N	110.547	0.027	1
1	A	84	GLY	CA	45.216	0.033	1
1	A	86	ALA	H	8.203	0.005	1
1	A	86	ALA	N	125.783	0.064	1
1	A	86	ALA	CA	51.982	0.045	1
1	A	86	ALA	CB	18.555	0.089	1
1	A	87	ARG	H	7.71	0.006	1
1	A	87	ARG	N	119.254	0.031	1
1	A	87	ARG	CB	31.882	0.011	1
1	A	87	ARG	CA	55.553	0.007	1
1	A	88	TYR	H	8.309	0.005	1
1	A	88	TYR	N	120.404	0.042	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	88	TYR	CB	38.586	0.016	1
1	A	88	TYR	CA	57.392	0.089	1
1	A	89	ARG	N	125.203	0.023	1
1	A	89	ARG	H	8.393	0.003	1
1	A	89	ARG	CA	54.651	0.081	1
1	A	89	ARG	CB	33.37	0.025	1
1	A	90	CYS	H	9.129	0.009	1
1	A	90	CYS	N	128.339	0.015	1
1	A	90	CYS	CB	29.565	0.061	1
1	A	90	CYS	CA	59.352	0.024	1
1	A	91	GLU	N	131.943	0.014	1
1	A	91	GLU	H	9.4	0.004	1
1	A	91	GLU	CA	58.609	0.006	1
1	A	91	GLU	CB	29.5	0.016	1
1	A	92	ASP	H	8.368	0.004	1
1	A	92	ASP	N	119.88	0.026	1
1	A	92	ASP	CB	40.971	.	1
1	A	92	ASP	CA	56.817	0.005	1
1	A	102	ASN	H	7.855	0.006	1
1	A	102	ASN	N	121.043	0.018	1
1	A	102	ASN	CA	55.094	0.028	1
1	A	102	ASN	CB	37.311	0.024	1
1	A	101	GLY	H	8.363	0.011	1
1	A	101	GLY	N	109.949	0.027	1
1	A	101	GLY	CA	46.724	0.007	1
1	A	100	SER	H	8.334	0.002	1
1	A	100	SER	N	117.319	0.029	1
1	A	100	SER	CB	61.869	0.035	1
1	A	100	SER	CA	60.247	0.034	1
1	A	99	THR	N	107.885	0.039	1
1	A	99	THR	H	7.057	0.005	1
1	A	99	THR	CB	72.938	0.092	1
1	A	99	THR	CA	58.596	0.042	1
1	A	98	THR	H	9.407	0.002	1
1	A	98	THR	N	110.822	0.045	1
1	A	98	THR	CA	63.186	0.082	1
1	A	98	THR	CB	69.667	0.038	1
1	A	97	PHE	H	8.698	0.005	1
1	A	97	PHE	N	118.189	0.029	1
1	A	97	PHE	CA	56.906	0.033	1
1	A	97	PHE	CB	43.308	0.03	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	96	LEU	H	7.583	0.003	1
1	A	96	LEU	N	119.809	0.041	1
1	A	96	LEU	CA	53.606	0.055	1
1	A	96	LEU	CB	44.703	0.055	1
1	A	95	LYS	H	7.736	0.003	1
1	A	95	LYS	N	121.988	0.032	1
1	A	95	LYS	CA	58.154	0.039	1
1	A	95	LYS	CB	33.907	0.035	1
1	A	94	GLY	N	113.91	0.023	1
1	A	94	GLY	H	8.297	0.003	1
1	A	94	GLY	CA	46.048	0.044	1
1	A	93	CYS	H	7.745	0.003	1
1	A	93	CYS	N	114.427	0.018	1
1	A	93	CYS	CA	58.485	0.034	1
1	A	93	CYS	CB	32.204	0.015	1
1	A	103	LEU	H	7.219	0.01	1
1	A	103	LEU	N	123.206	0.018	1
1	A	103	LEU	CA	57.987	0.024	1
1	A	103	LEU	CB	40.394	0.015	1
1	A	104	LYS	H	8.128	0.005	1
1	A	104	LYS	N	119.101	0.023	1
1	A	104	LYS	CA	59.259	0.046	1
1	A	104	LYS	CB	31.899	0.025	1
1	A	105	ARG	H	7.548	0.008	1
1	A	105	ARG	N	117.566	0.031	1
1	A	105	ARG	CB	30.096	0.031	1
1	A	105	ARG	CA	59.004	0.03	1
1	A	106	HIS	H	7.308	0.007	1
1	A	106	HIS	N	118.745	0.019	1
1	A	106	HIS	CB	27.92	0.029	1
1	A	106	HIS	CA	58.632	0.0	1
1	A	107	GLN	H	8.028	0.004	1
1	A	107	GLN	N	115.205	0.018	1
1	A	107	GLN	CB	28.192	0.032	1
1	A	107	GLN	CA	59.228	0.043	1
1	A	108	LEU	H	6.922	0.006	1
1	A	108	LEU	N	118.996	0.022	1
1	A	108	LEU	CA	57.065	0.076	1
1	A	108	LEU	CB	41.62	0.018	1
1	A	109	VAL	H	7.81	0.006	1
1	A	109	VAL	N	115.351	0.01	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	109	VAL	CA	63.691	0.076	1
1	A	109	VAL	CB	30.921	0.055	1
1	A	110	HIS	H	7.12	0.008	1
1	A	110	HIS	N	117.469	0.029	1
1	A	110	HIS	CA	54.637	0.027	1
1	A	110	HIS	CB	28.539	0.023	1
1	A	111	SER	H	7.586	0.008	1
1	A	111	SER	N	114.75	0.015	1
1	A	111	SER	CB	64.113	0.114	1
1	A	111	SER	CA	58.656	0.112	1
1	A	112	GLY	N	116.862	0.014	1
1	A	112	GLY	H	7.867	0.006	1
1	A	112	GLY	CA	46.214	0.016	1
1	A	60	TYR	H	7.713	0.018	1
1	A	60	TYR	N	118.143	0.225	1
1	A	60	TYR	CA	57.087	.	1
1	A	60	TYR	CB	38.36	0.018	1
1	A	59	PRO	CB	32.153	0.041	1
1	A	59	PRO	CA	63.362	0.036	1
1	A	61	GLY	H	8.403	0.004	1
1	A	61	GLY	N	112.201	0.039	1
1	A	61	GLY	CA	44.442	0.018	1
1	A	62	CYS	H	8.877	0.004	1
1	A	62	CYS	N	124.508	0.045	1
1	A	62	CYS	CA	59.136	0.038	1
1	A	62	CYS	CB	29.66	0.023	1
1	A	70	ARG	H	9.262	0.006	1
1	A	70	ARG	N	119.104	0.018	1
1	A	70	ARG	CA	57.832	0.011	1
1	A	70	ARG	CB	31.526	0.082	1
1	A	71	LEU	H	6.747	0.01	1
1	A	71	LEU	N	113.229	0.032	1
1	A	71	LEU	CA	52.603	0.015	1
1	A	71	LEU	CB	46.437	0.053	1
1	A	72	ILE	N	126.292	0.04	1
1	A	72	ILE	H	8.44	0.01	1
1	A	72	ILE	CA	63.425	0.037	1
1	A	72	ILE	CB	37.237	0.05	1
1	A	73	SER	N	115.339	0.015	1
1	A	73	SER	H	7.969	0.014	1
1	A	69	TYR	H	8.415	0.005	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	69	TYR	N	117.346	0.019	1
1	A	69	TYR	CB	44.55	0.018	1
1	A	69	TYR	CA	57.516	.	1
1	A	68	SER	H	7.671	0.005	1
1	A	68	SER	N	114.389	0.022	1
1	A	68	SER	CB	65.892	0.036	1
1	A	68	SER	CA	56.92	0.054	1
1	A	67	LYS	H	7.83	0.005	1
1	A	67	LYS	N	123.168	0.033	1
1	A	67	LYS	CA	57.857	0.014	1
1	A	67	LYS	CB	33.561	0.051	1
1	A	66	GLY	H	8.123	0.007	1
1	A	66	GLY	N	112.681	0.028	1
1	A	66	GLY	CA	46.009	0.021	1
1	A	65	CYS	H	7.859	0.008	1
1	A	65	CYS	N	114.678	0.026	1
1	A	65	CYS	CA	58.35	0.003	1
1	A	65	CYS	CB	32.324	0.037	1
1	A	64	GLU	H	8.557	0.004	1
1	A	64	GLU	N	120.454	0.025	1
1	A	64	GLU	CA	58.39	0.071	1
1	A	64	GLU	CB	29.568	0.026	1
1	A	10	GLY	H	8.072	0.005	1
1	A	10	GLY	N	113.426	0.055	1
1	A	10	GLY	CA	46.184	0.032	1
1	A	26	HIS	H	6.914	0.003	1
1	A	26	HIS	N	117.035	0.077	1
1	A	26	HIS	CA	55.499	.	1
1	A	26	HIS	CB	28.458	.	1
1	A	25	ILE	H	7.653	0.005	1
1	A	25	ILE	N	117.012	0.039	1
1	A	25	ILE	CA	63.271	.	1
1	A	25	ILE	CB	37.339	.	1
1	A	27	THR	N	111.784	0.029	1
1	A	27	THR	H	7.578	0.005	1
1	A	27	THR	CA	62.461	0.018	1
1	A	27	THR	CB	69.607	0.033	1
1	A	28	GLY	N	110.039	0.015	1
1	A	28	GLY	H	8.017	0.003	1
1	A	28	GLY	CA	45.298	0.056	1
1	A	29	GLU	N	119.56	0.021	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	29	GLU	H	7.842	0.003	1
1	A	29	GLU	CB	30.371	0.005	1
1	A	29	GLU	CA	56.712	0.043	1
1	A	24	ARG	H	6.697	0.007	1
1	A	24	ARG	N	118.44	0.029	1
1	A	24	ARG	CB	29.707	.	1
1	A	24	ARG	CA	57.78	.	1
1	A	23	ILE	H	7.605	0.004	1
1	A	23	ILE	N	111.694	0.039	1
1	A	23	ILE	CA	64.98	.	1
1	A	23	ILE	CB	36.77	.	1
1	A	22	HIS	H	7.546	0.005	1
1	A	22	HIS	N	118.837	0.047	1
1	A	22	HIS	CB	28.45	0.01	1
1	A	22	HIS	CA	59.445	.	1
1	A	21	ARG	H	7.438	0.007	1
1	A	21	ARG	N	117.022	0.051	1
1	A	21	ARG	CB	30.474	.	1
1	A	21	ARG	CA	58.98	.	1
1	A	20	LYS	H	8.249	0.007	1
1	A	20	LYS	N	117.574	0.054	1
1	A	20	LYS	CB	31.55	0.1	1
1	A	20	LYS	CA	59.281	.	1
1	A	19	PHE	H	7.912	0.027	1
1	A	19	PHE	N	122.914	0.161	1
1	A	19	PHE	CA	60.486	.	1
1	A	19	PHE	CB	39.212	.	1
1	A	4	HIS	H	8.489	0.005	1
1	A	4	HIS	N	125.506	0.191	1
1	A	4	HIS	CA	54.233	.	1
1	A	4	HIS	CB	30.216	0.027	1
1	A	5	LYS	N	124.514	0.074	1
1	A	5	LYS	H	8.472	0.004	1
1	A	5	LYS	CB	35.314	.	1
1	A	5	LYS	CA	54.572	.	1
1	A	6	CYS	H	9.165	0.007	1
1	A	6	CYS	N	128.563	0.044	1
1	A	6	CYS	CB	29.642	0.007	1
1	A	6	CYS	CA	59.537	.	1
1	A	7	GLU	N	132.438	0.018	1
1	A	7	GLU	H	9.7	0.005	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	GLU	CA	58.94	.	1
1	A	7	GLU	CB	29.785	.	1
1	A	75	LEU	CA	57.521	0.041	1
1	A	75	LEU	CB	40.133	0.049	1
1	A	9	CYS	N	115.054	0.047	1
1	A	9	CYS	H	7.905	0.006	1
1	A	9	CYS	CA	58.495	.	1
1	A	9	CYS	CB	32.163	0.03	1
1	A	8	ASP	H	8.348	0.015	1
1	A	8	ASP	N	119.728	0.01	1
1	A	73	SER	CA	60.781	0.036	1
1	A	73	SER	CB	60.779	0.038	1
1	A	3	ILE	C	174.793	.	1
1	A	4	HIS	C	173.614	.	1
1	A	5	LYS	C	175.057	.	1
1	A	6	CYS	C	177.449	.	1
1	A	7	GLU	C	176.609	.	1
1	A	8	ASP	C	176.809	.	1
1	A	9	CYS	C	176.131	.	1
1	A	20	LYS	C	180.33	.	1
1	A	19	PHE	C	175.66	.	1
1	A	21	ARG	C	178.038	.	1
1	A	22	HIS	C	176.764	.	1
1	A	23	ILE	C	177.744	.	1
1	A	24	ARG	C	178.454	.	1
1	A	25	ILE	C	177.463	.	1
1	A	26	HIS	C	175.839	.	1
1	A	27	THR	C	175.349	.	1
1	A	28	GLY	C	173.981	.	1
1	A	29	GLU	C	176.284	.	1
1	A	59	PRO	C	176.024	.	1
1	A	60	TYR	C	174.982	.	1
1	A	61	GLY	C	172.575	.	1
1	A	63	GLU	C	176.527	.	1
1	A	64	GLU	C	177.034	.	1
1	A	65	CYS	C	175.985	.	1
1	A	67	LYS	C	174.601	.	1
1	A	68	SER	C	172.719	.	1
1	A	69	TYR	C	175.527	.	1
1	A	70	ARG	C	174.748	.	1
1	A	71	LEU	C	177.289	.	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	72	ILE	C	176.755	.	1
1	A	73	SER	C	177.356	.	1
1	A	74	LEU	C	179.037	.	1
1	A	75	LEU	C	177.886	.	1
1	A	76	ASN	C	178.25	.	1
1	A	77	LEU	C	179.05	.	1
1	A	78	HIS	C	177.088	.	1
1	A	79	LYS	C	178.69	.	1
1	A	80	LYS	C	178.242	.	1
1	A	81	ARG	C	177.56	.	1
1	A	82	HIS	C	175.136	.	1
1	A	83	SER	C	174.884	.	1
1	A	84	GLY	C	173.863	.	1
1	A	85	GLU	C	176.025	.	1
1	A	86	ALA	C	176.399	.	1
1	A	87	ARG	C	175.255	.	1
1	A	88	TYR	C	173.868	.	1
1	A	89	ARG	C	175.014	.	1
1	A	90	CYS	C	176.979	.	1
1	A	91	GLU	C	176.617	.	1
1	A	92	ASP	C	176.863	.	1
1	A	93	CYS	C	176.057	.	1
1	A	94	GLY	C	173.535	.	1
1	A	95	LYS	C	173.898	.	1
1	A	96	LEU	C	176.419	.	1
1	A	97	PHE	C	176.114	.	1
1	A	98	THR	C	175.327	.	1
1	A	99	THR	C	173.724	.	1
1	A	100	SER	C	177.528	.	1
1	A	101	GLY	C	176.226	.	1
1	A	102	ASN	C	178.019	.	1
1	A	103	LEU	C	177.152	.	1
1	A	104	LYS	C	179.296	.	1
1	A	105	ARG	C	178.815	.	1
1	A	106	HIS	C	176.007	.	1
1	A	107	GLN	C	177.25	.	1
1	A	108	LEU	C	179.449	.	1
1	A	109	VAL	C	176.951	.	1
1	A	110	HIS	C	174.994	.	1
1	A	111	SER	C	173.908	.	1
1	A	3	ILE	CA	60.139	0.127	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	ILE	CB	39.322	.	1
1	A	8	ASP	CB	41.101	0.007	1
1	A	8	ASP	CA	56.93	.	1
1	A	18	ASN	CB	37.195	0.012	1
1	A	18	ASN	CA	55.408	.	1
1	A	108	LEU	CD1	25.023	0.014	2
1	A	108	LEU	CD2	22.692	0.022	2
1	A	107	GLN	CG	35.569	0.033	1
1	A	105	ARG	CG	27.603	0.039	1
1	A	105	ARG	CD	43.022	0.025	1
1	A	104	LYS	CE	41.911	0.007	1
1	A	104	LYS	CD	28.941	0.001	1
1	A	104	LYS	CG	25.183	0.059	1
1	A	20	LYS	CD	28.627	.	1
1	A	20	LYS	CG	26.01	.	1
1	A	29	GLU	CG	36.103	0.013	1
1	A	59	PRO	CD	50.14	0.03	1
1	A	59	PRO	CG	26.66	.	1
1	A	63	GLU	CG	36.115	0.031	1
1	A	64	GLU	CG	35.439	0.018	1
1	A	67	LYS	CE	41.334	.	1
1	A	67	LYS	CD	28.665	.	1
1	A	67	LYS	CG	26.102	.	1
1	A	70	ARG	CD	43.136	.	1
1	A	70	ARG	CG	27.922	0.003	1
1	A	72	ILE	CD1	13.265	0.057	1
1	A	72	ILE	CG2	16.818	0.043	1
1	A	79	LYS	CD	29.754	.	1
1	A	79	LYS	CG	26.57	.	1
1	A	80	LYS	CD	29.129	0.005	1
1	A	80	LYS	CG	25.12	0.001	1
1	A	81	ARG	CD	43.086	0.008	1
1	A	81	ARG	CG	26.896	0.015	1
1	A	85	GLU	CG	36.171	0.04	1
1	A	87	ARG	CD	43.104	0.119	1
1	A	87	ARG	CG	26.77	0.075	1
1	A	89	ARG	CD	43.296	0.027	1
1	A	89	ARG	CG	27.328	0.015	1
1	A	91	GLU	CG	35.993	0.022	1
1	A	95	LYS	CE	42.062	0.033	1
1	A	98	THR	CG2	22.457	0.038	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	112	GLY	HA2	3.643	0.017	1
1	A	112	GLY	HA3	3.643	0.015	1
1	A	111	SER	HA	4.328	0.006	1
1	A	110	HIS	HA	4.717	0.013	1
1	A	109	VAL	HA	3.772	0.006	1
1	A	108	LEU	HA	3.95	0.011	1
1	A	107	GLN	HA	3.455	0.004	1
1	A	106	HIS	HA	4.051	0.012	1
1	A	105	ARG	HA	3.844	0.008	1
1	A	104	LYS	HA	3.913	0.005	1
1	A	103	LEU	HA	3.031	0.004	1
1	A	102	ASN	HA	4.335	0.005	1
1	A	100	SER	HA	3.21	0.006	1
1	A	99	THR	HA	4.494	0.01	1
1	A	97	PHE	HA	4.672	0.009	1
1	A	96	LEU	HA	4.758	0.008	1
1	A	95	LYS	HA	3.841	0.004	1
1	A	94	GLY	HA3	4.091	0.013	2
1	A	94	GLY	HA2	3.574	0.005	2
1	A	93	CYS	HA	4.995	0.006	1
1	A	92	ASP	HA	4.349	0.009	1
1	A	91	GLU	HA	3.996	0.006	1
1	A	90	CYS	HA	4.43	0.005	1
1	A	89	ARG	HA	4.857	0.006	1
1	A	88	TYR	HA	4.447	0.007	1
1	A	87	ARG	HA	4.181	0.01	1
1	A	86	ALA	HA	4.105	0.007	1
1	A	85	GLU	HA	4.087	0.008	1
1	A	84	GLY	HA3	3.85	0.009	1
1	A	84	GLY	HA2	3.85	0.009	1
1	A	82	HIS	HA	4.693	0.005	1
1	A	81	ARG	HA	3.932	0.01	1
1	A	80	LYS	HA	3.929	0.009	1
1	A	78	HIS	HA	3.985	0.008	1
1	A	77	LEU	HA	3.907	0.006	1
1	A	76	ASN	HA	4.199	0.01	1
1	A	75	LEU	HA	3.466	0.004	1
1	A	74	LEU	HA	3.932	0.01	1
1	A	73	SER	HA	3.91	0.007	1
1	A	72	ILE	HA	3.158	0.009	1
1	A	71	LEU	HA	4.869	0.005	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	69	TYR	HA	4.535	0.01	1
1	A	68	SER	HA	5.12	0.01	1
1	A	67	LYS	HA	3.936	0.017	1
1	A	66	GLY	HA3	4.095	0.008	2
1	A	66	GLY	HA2	3.676	0.007	2
1	A	65	CYS	HA	4.991	0.008	1
1	A	64	GLU	HA	4.117	0.007	1
1	A	62	CYS	HA	4.339	0.017	1
1	A	60	TYR	HA	4.601	0.004	1
1	A	29	GLU	HA	4.012	0.005	1
1	A	26	HIS	HA	4.644	.	1
1	A	25	ILE	HA	3.724	.	1
1	A	21	ARG	HA	3.742	.	1
1	A	10	GLY	HA3	4.116	.	2
1	A	10	GLY	HA2	3.639	.	2
1	A	9	CYS	HA	5.021	.	1
1	A	8	ASP	HA	4.367	.	1
1	A	7	GLU	HA	3.973	.	1
1	A	6	CYS	HA	4.462	.	1
1	A	5	LYS	HA	4.848	.	1
1	A	4	HIS	HA	4.288	.	1
1	A	110	HIS	HB3	3.14	0.006	2
1	A	110	HIS	HB2	3.019	0.01	2
1	A	109	VAL	HB	1.782	0.003	1
1	A	109	VAL	HG11	0.486	0.003	2
1	A	109	VAL	HG12	0.486	0.003	2
1	A	109	VAL	HG13	0.486	0.003	2
1	A	109	VAL	HG21	0.312	0.006	2
1	A	109	VAL	HG22	0.312	0.006	2
1	A	109	VAL	HG23	0.312	0.006	2
1	A	109	VAL	CG2	19.649	0.006	2
1	A	109	VAL	CG1	19.276	0.152	2
1	A	108	LEU	HG	1.686	0.005	1
1	A	108	LEU	HB3	1.588	0.009	2
1	A	108	LEU	HB2	1.356	0.005	2
1	A	108	LEU	HD21	0.797	0.006	2
1	A	108	LEU	HD22	0.797	0.006	2
1	A	108	LEU	HD23	0.797	0.006	2
1	A	108	LEU	HD11	0.715	0.009	2
1	A	108	LEU	HD12	0.715	0.009	2
1	A	108	LEU	HD13	0.715	0.009	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	108	LEU	CG	26.637	0.0	1
1	A	107	GLN	HG3	2.699	0.008	2
1	A	107	GLN	HG2	2.642	0.006	2
1	A	107	GLN	HB3	2.126	0.007	2
1	A	107	GLN	HB2	2.056	0.007	2
1	A	106	HIS	HB3	2.816	0.01	2
1	A	106	HIS	HB2	2.587	0.006	2
1	A	104	LYS	HE2	2.782	0.002	1
1	A	104	LYS	HE3	2.782	0.002	1
1	A	104	LYS	HB2	1.676	0.004	1
1	A	104	LYS	HB3	1.676	0.004	1
1	A	104	LYS	HG3	1.344	0.002	2
1	A	104	LYS	HG2	1.264	0.003	2
1	A	104	LYS	HD2	1.486	0.004	1
1	A	104	LYS	HD3	1.486	0.004	1
1	A	103	LEU	HB3	1.825	0.004	2
1	A	103	LEU	HB2	1.135	0.005	2
1	A	103	LEU	CG	26.902	.	1
1	A	103	LEU	HG	1.305	0.008	1
1	A	103	LEU	CD2	26.391	0.022	2
1	A	103	LEU	HD21	0.877	0.009	2
1	A	103	LEU	HD22	0.877	0.009	2
1	A	103	LEU	HD23	0.877	0.009	2
1	A	103	LEU	CD1	22.93	0.086	2
1	A	103	LEU	HD11	0.813	0.007	2
1	A	103	LEU	HD12	0.813	0.007	2
1	A	103	LEU	HD13	0.813	0.007	2
1	A	102	ASN	HB3	2.814	0.009	2
1	A	102	ASN	HB2	2.722	0.011	2
1	A	100	SER	HB3	3.368	0.004	2
1	A	100	SER	HB2	3.527	0.006	2
1	A	99	THR	HB	4.301	0.005	1
1	A	99	THR	HG21	1.084	0.006	1
1	A	99	THR	HG22	1.084	0.006	1
1	A	99	THR	HG23	1.084	0.006	1
1	A	98	THR	HA	4.481	0.013	1
1	A	98	THR	HB	4.345	0.003	1
1	A	98	THR	HG21	1.131	0.005	1
1	A	98	THR	HG22	1.131	0.005	1
1	A	98	THR	HG23	1.131	0.005	1
1	A	97	PHE	HB3	3.115	0.007	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	97	PHE	HB2	2.663	0.009	2
1	A	96	LEU	HB3	1.32	0.009	2
1	A	96	LEU	HB2	1.06	0.01	2
1	A	96	LEU	CD2	24.998	0.039	2
1	A	96	LEU	HD11	0.69	0.011	2
1	A	96	LEU	HD12	0.69	0.011	2
1	A	96	LEU	HD13	0.69	0.011	2
1	A	96	LEU	CD1	23.527	0.021	2
1	A	96	LEU	HD21	0.565	0.006	2
1	A	96	LEU	HD22	0.565	0.006	2
1	A	96	LEU	HD23	0.565	0.006	2
1	A	96	LEU	CG	26.833	0.024	1
1	A	96	LEU	HG	1.426	0.001	1
1	A	95	LYS	HB3	1.269	0.005	2
1	A	95	LYS	HB2	1.192	0.007	2
1	A	95	LYS	HE3	2.822	0.004	1
1	A	95	LYS	HE2	2.822	0.004	1
1	A	95	LYS	CD	29.222	0.025	1
1	A	95	LYS	HD3	1.344	0.002	2
1	A	95	LYS	HD2	1.405	0.007	2
1	A	95	LYS	CG	26.788	0.018	1
1	A	95	LYS	HG3	1.03	0.006	2
1	A	95	LYS	HG2	1.415	0.009	2
1	A	93	CYS	HB3	3.286	0.007	2
1	A	93	CYS	HB2	2.751	0.006	2
1	A	92	ASP	HB3	3.178	.	2
1	A	92	ASP	HB2	3.11	.	2
1	A	91	GLU	HG3	2.261	0.004	2
1	A	91	GLU	HG2	2.218	0.004	2
1	A	91	GLU	HB3	1.997	0.004	2
1	A	91	GLU	HB2	1.891	0.001	2
1	A	90	CYS	HB3	3.259	0.005	2
1	A	90	CYS	HB2	2.732	0.005	2
1	A	88	TYR	HB3	2.754	0.01	2
1	A	88	TYR	HB2	2.642	0.009	2
1	A	86	ALA	HB1	1.071	0.005	1
1	A	86	ALA	HB2	1.071	0.005	1
1	A	86	ALA	HB3	1.071	0.005	1
1	A	85	GLU	HG3	2.125	0.011	2
1	A	85	GLU	HG2	2.083	0.008	2
1	A	85	GLU	HB3	1.857	0.012	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	85	GLU	HB2	1.796	0.008	2
1	A	83	SER	HA	4.309	0.016	1
1	A	83	SER	HB2	3.166	0.007	1
1	A	83	SER	HB3	3.166	0.007	1
1	A	82	HIS	HB3	3.137	0.012	2
1	A	82	HIS	HB2	3.016	0.007	2
1	A	77	LEU	CG	26.561	0.004	1
1	A	77	LEU	HG	1.547	0.007	1
1	A	77	LEU	HB3	1.559	0.008	2
1	A	77	LEU	HB2	1.433	0.01	2
1	A	77	LEU	CD2	24.569	0.006	2
1	A	77	LEU	HD21	0.737	0.007	2
1	A	77	LEU	HD22	0.737	0.007	2
1	A	77	LEU	HD23	0.737	0.007	2
1	A	77	LEU	CD1	23.497	0.03	2
1	A	77	LEU	HD11	0.719	0.01	2
1	A	77	LEU	HD12	0.719	0.01	2
1	A	77	LEU	HD13	0.719	0.01	2
1	A	99	THR	CG2	21.737	0.026	1
1	A	80	LYS	HB3	1.714	0.007	1
1	A	80	LYS	HB2	1.714	0.007	1
1	A	80	LYS	HD3	1.526	0.001	1
1	A	80	LYS	HD2	1.526	0.001	1
1	A	80	LYS	HE2	2.822	0.005	1
1	A	80	LYS	HE3	2.821	0.008	1
1	A	80	LYS	HG3	1.355	0.009	2
1	A	80	LYS	HG2	1.265	0.001	2
1	A	76	ASN	HB2	2.57	0.005	1
1	A	76	ASN	HB3	2.57	0.005	1
1	A	75	LEU	HB3	1.856	0.006	2
1	A	75	LEU	HB2	1.256	0.008	2
1	A	75	LEU	CD2	26.274	0.011	2
1	A	75	LEU	HD21	0.858	0.014	2
1	A	75	LEU	HD22	0.858	0.014	2
1	A	75	LEU	HD23	0.858	0.014	2
1	A	75	LEU	CD1	22.622	0.025	2
1	A	75	LEU	HD11	0.886	0.01	2
1	A	75	LEU	HD12	0.886	0.01	2
1	A	75	LEU	HD13	0.886	0.01	2
1	A	74	LEU	CD1	26.116	0.043	2
1	A	74	LEU	HD21	1.044	0.008	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	74	LEU	HD22	1.044	0.008	2
1	A	74	LEU	HD23	1.044	0.008	2
1	A	74	LEU	CD2	22.105	0.011	2
1	A	74	LEU	HD11	0.768	0.007	2
1	A	74	LEU	HD12	0.768	0.007	2
1	A	74	LEU	HD13	0.768	0.007	2
1	A	74	LEU	CG	26.654	0.014	1
1	A	74	LEU	HG	1.552	0.006	1
1	A	74	LEU	HB3	1.75	0.011	2
1	A	74	LEU	HB2	1.292	0.015	2
1	A	72	ILE	HB	0.881	0.01	1
1	A	72	ILE	CG1	29.038	0.053	1
1	A	72	ILE	HG13	0.787	0.012	2
1	A	72	ILE	HG12	0.713	0.009	2
1	A	72	ILE	HG21	0.58	0.008	1
1	A	72	ILE	HG22	0.58	0.008	1
1	A	72	ILE	HG23	0.58	0.008	1
1	A	72	ILE	HD11	0.562	0.011	1
1	A	72	ILE	HD12	0.562	0.011	1
1	A	72	ILE	HD13	0.562	0.011	1
1	A	71	LEU	HB3	1.649	0.005	2
1	A	71	LEU	HB2	1.348	0.01	2
1	A	71	LEU	CD1	23.12	0.02	2
1	A	71	LEU	HD11	0.92	0.009	2
1	A	71	LEU	HD12	0.92	0.009	2
1	A	71	LEU	HD13	0.92	0.009	2
1	A	71	LEU	CD2	25.14	0.05	2
1	A	71	LEU	HD21	0.812	0.011	2
1	A	71	LEU	HD22	0.812	0.011	2
1	A	71	LEU	HD23	0.812	0.011	2
1	A	71	LEU	CG	25.055	0.069	1
1	A	71	LEU	HG	1.476	0.007	1
1	A	69	TYR	HB3	3.062	0.007	2
1	A	69	TYR	HB2	2.52	0.012	2
1	A	68	SER	HB3	3.491	0.006	2
1	A	68	SER	HB2	3.342	0.01	2
1	A	65	CYS	HB3	3.285	0.007	2
1	A	65	CYS	HB2	2.75	0.003	2
1	A	64	GLU	HG3	1.761	0.004	2
1	A	64	GLU	HG2	1.61	0.007	2
1	A	64	GLU	HB3	1.387	0.016	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	62	CYS	HB3	3.229	0.01	2
1	A	62	CYS	HB2	2.667	0.01	2
1	A	60	TYR	HB3	2.62	0.007	2
1	A	60	TYR	HB2	2.841	0.007	2
1	A	101	GLY	HA3	3.635	0.01	2
1	A	101	GLY	HA2	3.569	0.009	2
1	A	59	PRO	HA	4.066	0.005	1
1	A	59	PRO	HD3	3.394	0.004	2
1	A	59	PRO	HD2	3.434	0.007	2
1	A	59	PRO	HB3	0.976	0.002	2
1	A	59	PRO	HB2	0.919	0.004	2
1	A	59	PRO	HG3	1.799	0.007	2
1	A	59	PRO	HG2	1.568	0.006	2
1	A	89	ARG	HD3	2.957	0.008	2
1	A	89	ARG	HD2	2.932	0.005	2
1	A	89	ARG	HB3	1.604	0.006	2
1	A	89	ARG	HB2	1.291	0.009	2
1	A	89	ARG	HG2	1.099	0.006	1
1	A	89	ARG	HG3	1.099	0.006	1
1	A	87	ARG	HD3	2.85	0.005	2
1	A	87	ARG	HD2	2.929	0.007	2
1	A	87	ARG	HB3	1.36	0.009	1
1	A	87	ARG	HB2	1.36	0.009	1
1	A	87	ARG	HG3	1.201	0.008	2
1	A	87	ARG	HG2	1.13	0.008	2
1	A	79	LYS	HB3	1.816	0.013	1
1	A	79	LYS	HB2	1.816	0.012	1
1	A	79	LYS	HA	3.472	0.009	1
1	A	79	LYS	HE3	3.084	0.004	2
1	A	79	LYS	HE2	2.952	0.01	2
1	A	67	LYS	HB3	1.219	0.005	1
1	A	67	LYS	HB2	1.219	0.005	1
1	A	105	ARG	HD3	3.048	0.008	1
1	A	105	ARG	HD2	3.048	0.008	1
1	A	105	ARG	HG3	1.571	0.005	2
1	A	105	ARG	HG2	1.443	0.007	2
1	A	105	ARG	HB2	1.665	0.005	1
1	A	105	ARG	HB3	1.665	0.005	1
1	A	81	ARG	HD3	2.956	0.006	1
1	A	81	ARG	HD2	2.956	0.006	1
1	A	81	ARG	HB3	1.487	0.009	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	81	ARG	HB2	1.373	0.01	2
1	A	81	ARG	HG2	1.327	0.007	1
1	A	81	ARG	HG3	1.327	0.008	1
1	A	70	ARG	HA	4.323	0.009	1
1	A	70	ARG	HB2	1.813	0.007	1
1	A	70	ARG	HB3	1.812	0.007	1
1	A	70	ARG	HG3	1.666	0.008	1
1	A	70	ARG	HG2	1.665	0.007	1
1	A	64	GLU	HB2	1.351	0.009	2
1	A	61	GLY	HA3	3.421	0.003	2
1	A	61	GLY	HA2	4.532	0.003	2
1	A	80	LYS	CE	42.012	0.003	1
1	A	78	HIS	HB3	3.199	0.006	2
1	A	78	HIS	HB2	2.85	0.011	2
1	A	110	HIS	HD2	6.612	0.007	1
1	A	110	HIS	HE1	7.852	0.007	1
1	A	110	HIS	CD2	131.513	0.003	1
1	A	110	HIS	CE1	142.388	.	1
1	A	106	HIS	HD2	6.683	0.004	1
1	A	106	HIS	CD2	129.849	0.071	1
1	A	78	HIS	HD2	6.725	0.004	1
1	A	78	HIS	CD2	129.405	0.024	1
1	A	82	HIS	HD2	6.608	0.002	1
1	A	82	HIS	CD2	131.048	.	1
1	A	82	HIS	HE1	7.861	0.011	1
1	A	82	HIS	CE1	142.435	.	1
1	A	97	PHE	CD1	135.179	0.014	3
1	A	97	PHE	CD2	135.179	0.014	3
1	A	97	PHE	HD1	7.106	0.008	3
1	A	97	PHE	HD2	7.106	0.008	3
1	A	97	PHE	HE1	6.681	0.003	3
1	A	97	PHE	HE2	6.681	0.003	3
1	A	97	PHE	CE1	132.823	0.0	3
1	A	97	PHE	CE2	132.823	0.0	3
1	A	97	PHE	HZ	5.912	0.005	1
1	A	97	PHE	CZ	130.946	0.003	1
1	A	88	TYR	HD1	6.813	0.007	3
1	A	88	TYR	HD2	6.813	0.007	3
1	A	88	TYR	CD1	136.039	0.022	3
1	A	88	TYR	CD2	136.039	0.022	3
1	A	88	TYR	HE1	6.67	0.004	3

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	88	TYR	HE2	6.67	0.004	3
1	A	88	TYR	CE1	120.403	0.0	3
1	A	88	TYR	CE2	120.403	0.0	3
1	A	69	TYR	HD1	6.901	0.007	3
1	A	69	TYR	HD2	6.901	0.007	3
1	A	69	TYR	CD1	135.736	0.013	3
1	A	69	TYR	CD2	135.736	0.013	3
1	A	69	TYR	HE1	6.137	0.005	3
1	A	69	TYR	HE2	6.137	0.005	3
1	A	69	TYR	CE1	120.112	0.007	3
1	A	69	TYR	CE2	120.112	0.007	3
1	A	60	TYR	CD1	135.991	0.052	3
1	A	60	TYR	CD2	135.991	0.052	3
1	A	60	TYR	HD1	6.827	0.004	3
1	A	60	TYR	HD2	6.827	0.004	3
1	A	60	TYR	HE1	6.758	0.004	3
1	A	60	TYR	HE2	6.758	0.004	3
1	A	60	TYR	CE1	120.963	0.031	3
1	A	60	TYR	CE2	120.963	0.031	3
1	A	27	THR	CG2	21.598	.	1
1	A	27	THR	HG21	1.058	0.003	1
1	A	27	THR	HG22	1.058	0.003	1
1	A	27	THR	HG23	1.058	0.003	1
1	A	27	THR	HA	4.109	0.004	1
1	A	27	THR	HB	4.117	0.003	1
1	A	28	GLY	HA3	3.786	0.022	1
1	A	28	GLY	HA2	3.786	0.022	1
1	A	29	GLU	HB3	1.832	0.005	2
1	A	29	GLU	HB2	1.801	0.006	2
1	A	29	GLU	HG3	2.045	0.012	2
1	A	29	GLU	HG2	2.104	0.003	2
1	A	63	GLU	H	9.642	0.015	1
1	A	63	GLU	N	132.211	.	1
1	A	63	GLU	CB	29.324	0.018	1
1	A	63	GLU	CA	58.868	0.059	1
1	A	63	GLU	HB3	1.998	0.002	2
1	A	63	GLU	HB2	1.944	0.002	2
1	A	63	GLU	HG2	2.26	0.002	1
1	A	63	GLU	HG3	2.261	0.002	1
1	A	63	GLU	HA	4.012	0.001	1
1	A	79	LYS	CE	41.886	0.034	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	76	ASN	HD22	7.306	0.004	1
1	A	76	ASN	ND2	110.148	0.044	1
1	A	76	ASN	HD21	6.589	0.008	1
1	A	107	GLN	HE22	7.496	0.004	1
1	A	107	GLN	NE2	113.055	0.009	1
1	A	107	GLN	HE21	6.927	0.002	1
1	A	102	ASN	HD22	7.017	0.003	1
1	A	102	ASN	ND2	111.881	0.01	1
1	A	102	ASN	HD21	6.802	0.007	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	102	-0.07 ± 0.46	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	94	0.29 ± 0.27	None needed (< 0.5 ppm)
$^{13}\text{C}'$	91	0.05 ± 0.24	None needed (< 0.5 ppm)
^{15}N	96	-0.06 ± 0.58	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 74%, i.e. 224 atoms were assigned a chemical shift out of a possible 303. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	112/121 (93%)	45/48 (94%)	45/50 (90%)	22/23 (96%)
Sidechain	99/148 (67%)	62/95 (65%)	37/47 (79%)	0/6 (0%)
Aromatic	13/34 (38%)	7/18 (39%)	6/14 (43%)	0/2 (0%)
Overall	224/303 (74%)	114/161 (71%)	88/111 (79%)	22/31 (71%)

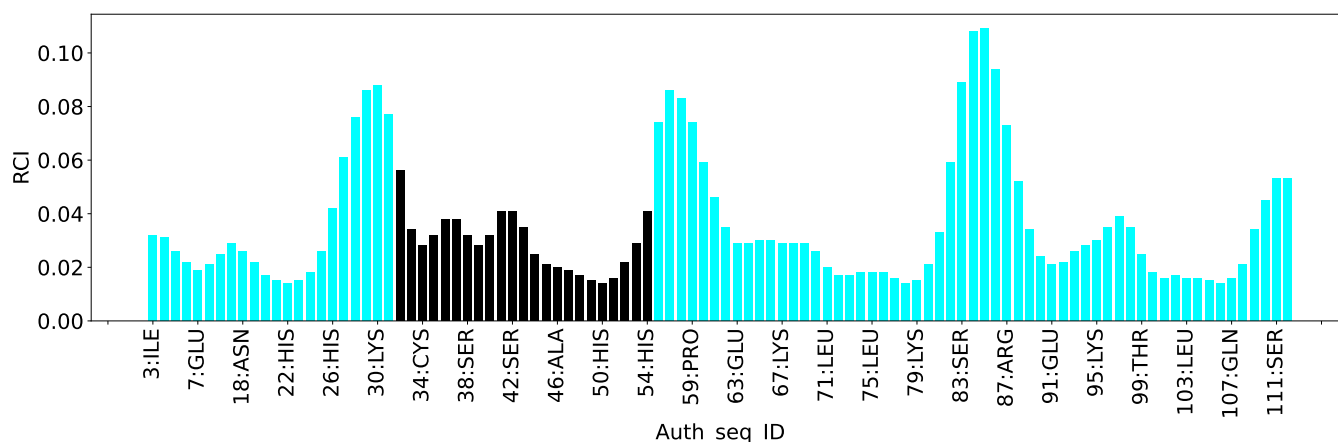
7.1.4 Statistically unusual chemical shifts ⓘ

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	439
Intra-residue ($ i-j =0$)	225
Sequential ($ i-j =1$)	108
Medium range ($ i-j >1$ and $ i-j <5$)	65
Long range ($ i-j \geq 5$)	41
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	50
Number of unmapped restraints	0
Number of restraints per residue	4.3
Number of long range restraints per residue ¹	0.4

¹Long 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)	7.2	0.2
0.2-0.5 (Medium)	5.1	0.5
>0.5 (Large)	1.5	2.25

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)	2.1	3.88
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

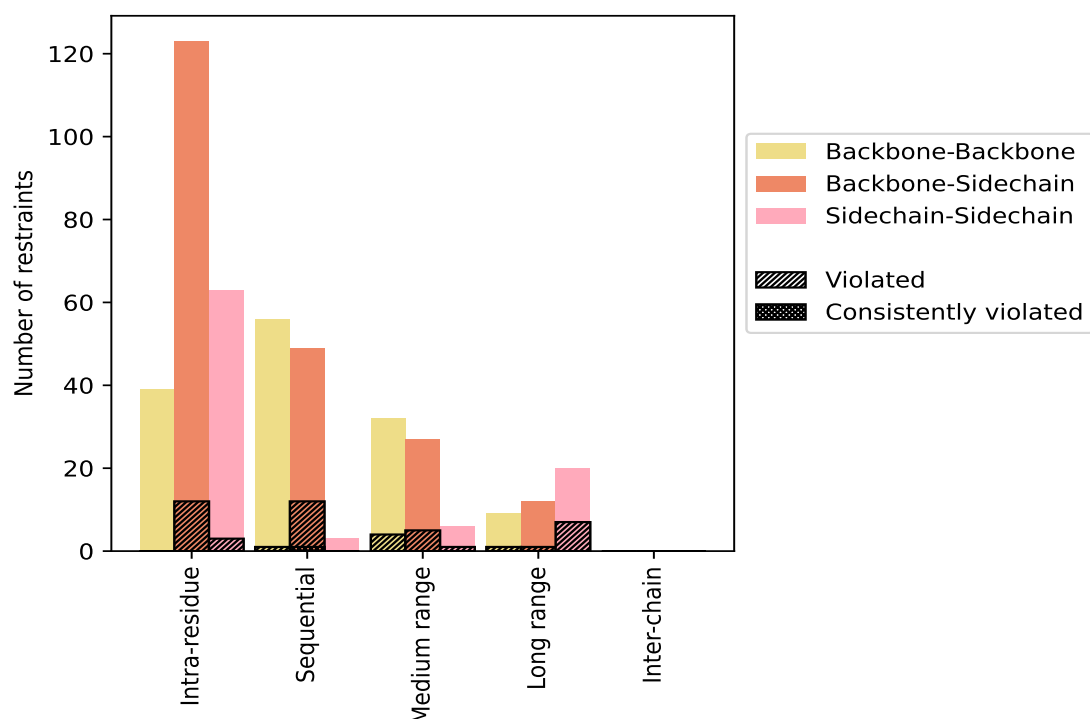
9.1 Summary of distance violations ⓘ

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	225	51.3	15	6.7	3.4	0	0.0	0.0
Backbone-Backbone	39	8.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	123	28.0	12	9.8	2.7	0	0.0	0.0
Sidechain-Sidechain	63	14.4	3	4.8	0.7	0	0.0	0.0
Sequential (i-j =1)	108	24.6	13	12.0	3.0	1	0.9	0.2
Backbone-Backbone	56	12.8	1	1.8	0.2	0	0.0	0.0
Backbone-Sidechain	49	11.2	12	24.5	2.7	1	2.0	0.2
Sidechain-Sidechain	3	0.7	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	65	14.8	10	15.4	2.3	0	0.0	0.0
Backbone-Backbone	32	7.3	4	12.5	0.9	0	0.0	0.0
Backbone-Sidechain	27	6.2	5	18.5	1.1	0	0.0	0.0
Sidechain-Sidechain	6	1.4	1	16.7	0.2	0	0.0	0.0
Long range (i-j ≥5)	41	9.3	9	22.0	2.1	0	0.0	0.0
Backbone-Backbone	9	2.1	1	11.1	0.2	0	0.0	0.0
Backbone-Sidechain	12	2.7	1	8.3	0.2	0	0.0	0.0
Sidechain-Sidechain	20	4.6	7	35.0	1.6	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	439	100.0	47	10.7	10.7	1	0.2	0.2
Backbone-Backbone	136	31.0	6	4.4	1.4	0	0.0	0.0
Backbone-Sidechain	211	48.1	30	14.2	6.8	1	0.5	0.2
Sidechain-Sidechain	92	21.0	11	12.0	2.5	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 [i](#)



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

9.2 Distance violation statistics for each model [i](#)

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	5	7	4	3	0	19	0.3	0.86	0.2	0.26
2	6	4	7	3	0	20	0.36	1.72	0.38	0.22
3	3	4	2	2	0	11	0.31	0.82	0.21	0.24
4	5	4	4	1	0	14	0.26	0.68	0.14	0.2
5	4	4	3	1	0	12	0.29	1.32	0.32	0.2
6	3	4	4	1	0	12	0.2	0.44	0.11	0.15
7	7	5	3	1	0	16	0.34	1.82	0.41	0.21
8	4	4	2	1	0	11	0.29	0.71	0.2	0.2
9	6	4	4	1	0	15	0.28	0.79	0.21	0.18
10	4	7	3	1	0	15	0.3	1.33	0.31	0.21

Continued on next page...

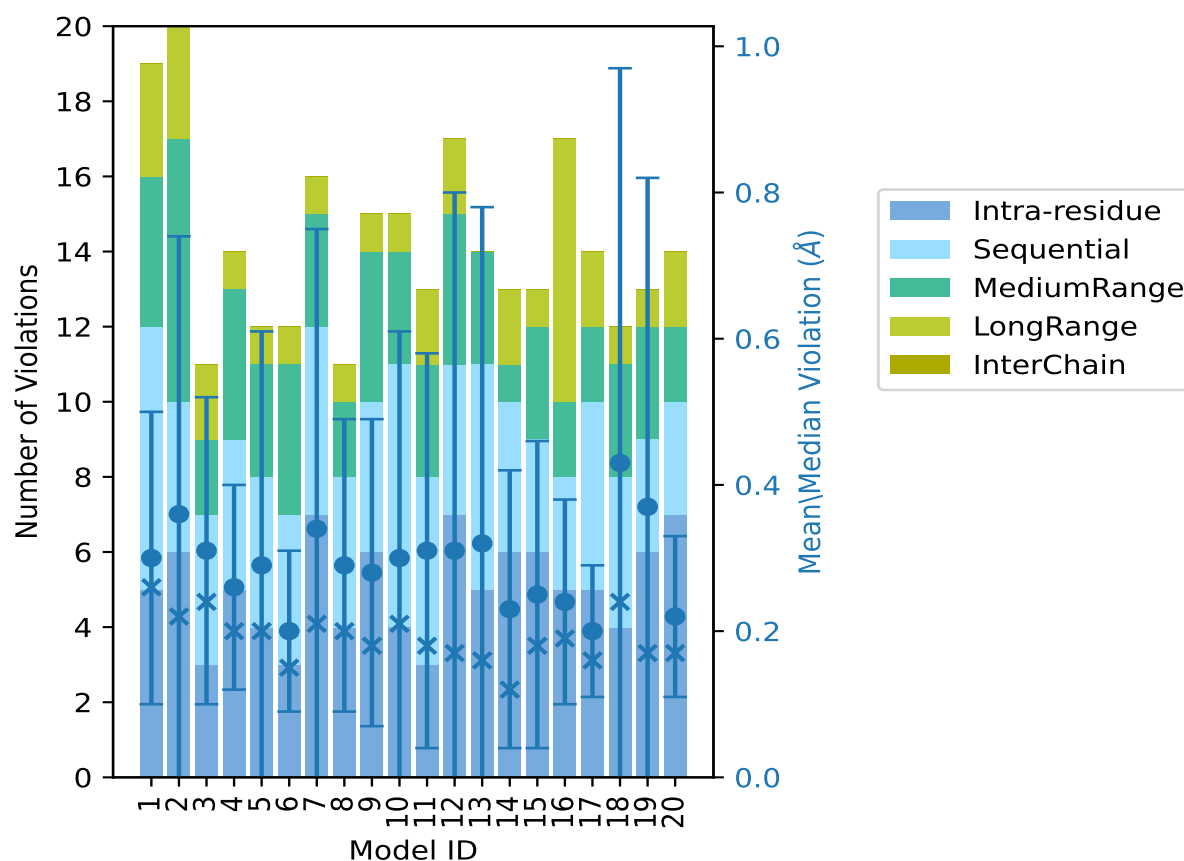
Continued from previous page...

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	3	5	3	2	0	13	0.31	1.01	0.27	0.18
12	7	4	4	2	0	17	0.31	2.25	0.49	0.17
13	5	6	3	0	0	14	0.32	1.95	0.46	0.16
14	6	4	1	2	0	13	0.23	0.83	0.19	0.12
15	6	3	3	1	0	13	0.25	0.91	0.21	0.18
16	5	3	2	7	0	17	0.24	0.62	0.14	0.19
17	5	5	2	2	0	14	0.2	0.39	0.09	0.16
18	4	4	3	1	0	12	0.43	2.17	0.54	0.24
19	6	3	3	1	0	13	0.37	1.81	0.45	0.17
20	7	3	2	2	0	14	0.22	0.43	0.11	0.17

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard 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

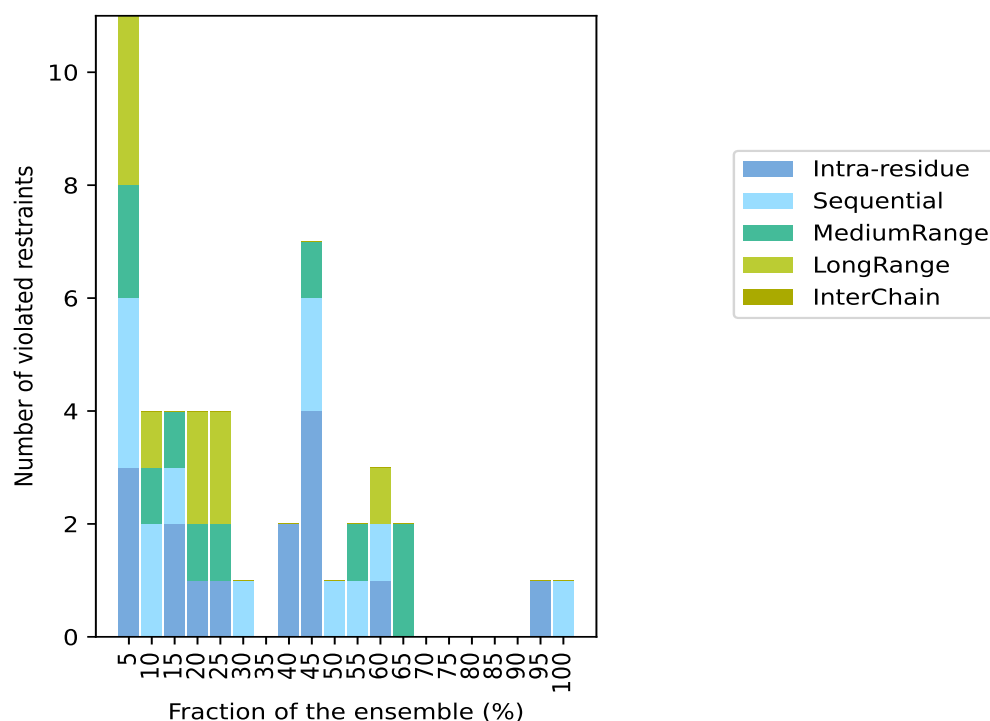
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 392(IR:210, SQ:95, MR:55, LR:32, IC:0) restraints are not 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	%
3	3	2	3	0	11	1	5.0
0	2	1	1	0	4	2	10.0
2	1	1	0	0	4	3	15.0
1	0	1	2	0	4	4	20.0
1	0	1	2	0	4	5	25.0
0	1	0	0	0	1	6	30.0
0	0	0	0	0	0	7	35.0
2	0	0	0	0	2	8	40.0
4	2	1	0	0	7	9	45.0
0	1	0	0	0	1	10	50.0
0	1	1	0	0	2	11	55.0
1	1	0	1	0	3	12	60.0
0	0	2	0	0	2	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
1	0	0	0	0	1	19	95.0
0	1	0	0	0	1	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

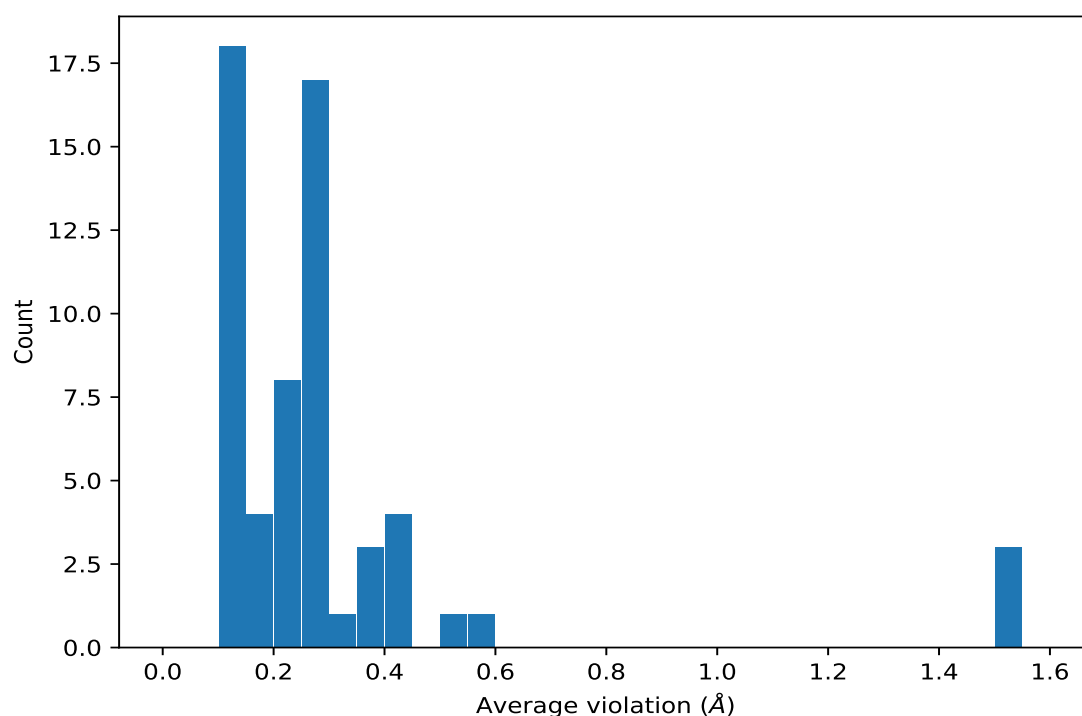
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

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 [i](#)

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.

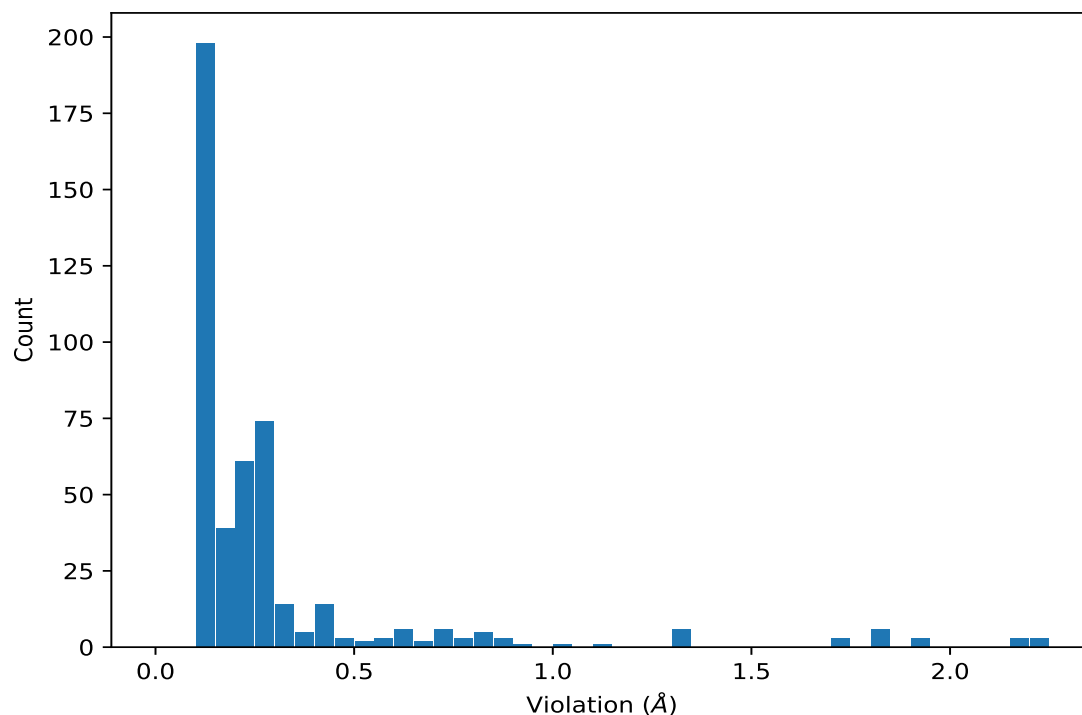
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,333)	1:45:A:ALA:H	1:46:A:ALA:HB1	20	0.14	0.01	0.13
(1,333)	1:45:A:ALA:H	1:46:A:ALA:HB2	20	0.14	0.01	0.13
(1,333)	1:45:A:ALA:H	1:46:A:ALA:HB3	20	0.14	0.01	0.13
(1,242)	1:57:A:LEU:H	1:57:A:LEU:HB3	19	0.21	0.04	0.21
(1,77)	1:47:A:CYS:HB3	1:43:A:ASP:H	13	0.37	0.17	0.36
(1,237)	1:45:A:ALA:HB1	1:43:A:ASP:HB2	13	0.14	0.03	0.14
(1,237)	1:45:A:ALA:HB2	1:43:A:ASP:HB2	13	0.14	0.03	0.14
(1,237)	1:45:A:ALA:HB3	1:43:A:ASP:HB2	13	0.14	0.03	0.14
(1,376)	1:36:A:GLU:HG3	1:54:A:HIS:HB2	12	0.58	0.28	0.56
(1,437)	1:56:A:PRO:HG2	1:57:A:LEU:H	12	0.32	0.11	0.32
(1,32)	1:43:A:ASP:H	1:43:A:ASP:HB3	12	0.12	0.02	0.12
(1,65)	1:57:A:LEU:HD11	1:53:A:THR:H	11	1.51	0.54	1.72
(1,65)	1:57:A:LEU:HD12	1:53:A:THR:H	11	1.51	0.54	1.72
(1,65)	1:57:A:LEU:HD13	1:53:A:THR:H	11	1.51	0.54	1.72
(1,260)	1:58:A:LYS:H	1:57:A:LEU:HB3	11	0.41	0.19	0.4
(1,435)	1:49:A:ALA:H	1:48:A:LYS:H	10	0.14	0.02	0.15

¹Number of violated models, ²Standard 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)
(1,65)	1:57:A:LEU:HD11	1:53:A:THR:H	12	2.25
(1,65)	1:57:A:LEU:HD12	1:53:A:THR:H	12	2.25
(1,65)	1:57:A:LEU:HD13	1:53:A:THR:H	12	2.25
(1,65)	1:57:A:LEU:HD11	1:53:A:THR:H	18	2.17
(1,65)	1:57:A:LEU:HD12	1:53:A:THR:H	18	2.17
(1,65)	1:57:A:LEU:HD13	1:53:A:THR:H	18	2.17
(1,65)	1:57:A:LEU:HD11	1:53:A:THR:H	13	1.95
(1,65)	1:57:A:LEU:HD12	1:53:A:THR:H	13	1.95

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,65)	1:57:A:LEU:HD13	1:53:A:THR:H	13	1.95
(1,65)	1:57:A:LEU:HD11	1:53:A:THR:H	7	1.82
(1,65)	1:57:A:LEU:HD12	1:53:A:THR:H	7	1.82
(1,65)	1:57:A:LEU:HD13	1:53:A:THR:H	7	1.82
(1,65)	1:57:A:LEU:HD11	1:53:A:THR:H	19	1.81
(1,65)	1:57:A:LEU:HD12	1:53:A:THR:H	19	1.81
(1,65)	1:57:A:LEU:HD13	1:53:A:THR:H	19	1.81
(1,65)	1:57:A:LEU:HD11	1:53:A:THR:H	2	1.72
(1,65)	1:57:A:LEU:HD12	1:53:A:THR:H	2	1.72
(1,65)	1:57:A:LEU:HD13	1:53:A:THR:H	2	1.72
(1,65)	1:57:A:LEU:HD11	1:53:A:THR:H	10	1.33
(1,65)	1:57:A:LEU:HD12	1:53:A:THR:H	10	1.33
(1,65)	1:57:A:LEU:HD13	1:53:A:THR:H	10	1.33
(1,65)	1:57:A:LEU:HD11	1:53:A:THR:H	5	1.32
(1,65)	1:57:A:LEU:HD12	1:53:A:THR:H	5	1.32
(1,65)	1:57:A:LEU:HD13	1:53:A:THR:H	5	1.32
(1,376)	1:36:A:GLU:HG3	1:54:A:HIS:HB2	2	1.13
(1,276)	1:37:A:CYS:H	1:36:A:GLU:HG3	11	1.01

10 Dihedral-angle violation analysis [i](#)

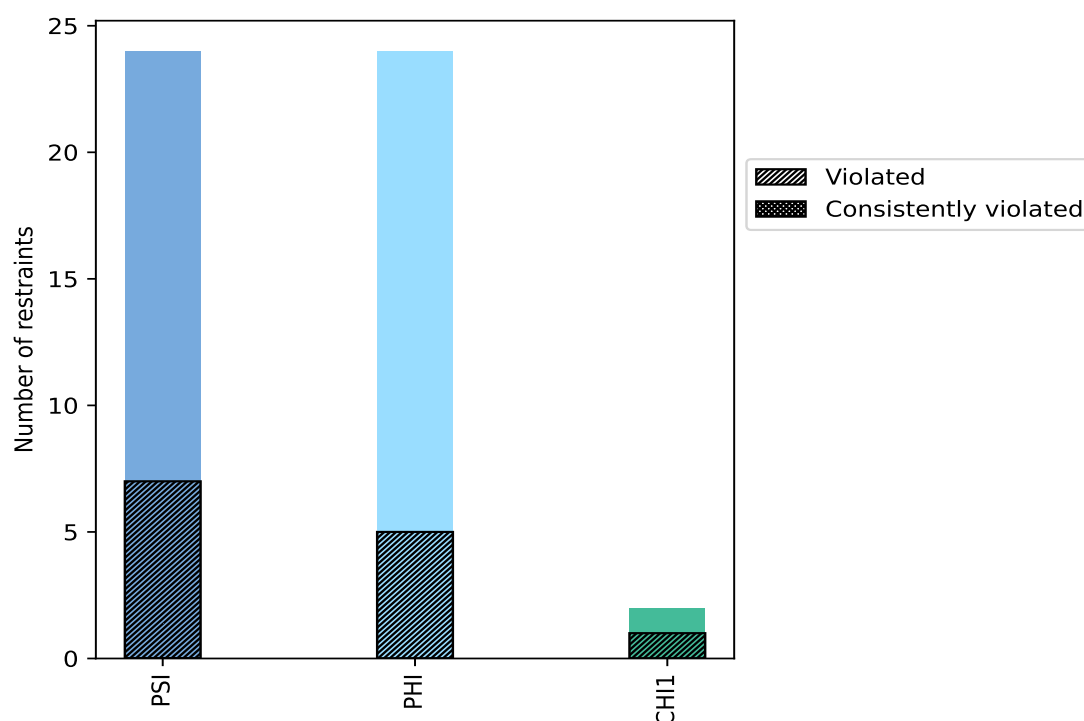
10.1 Summary of dihedral-angle violations [i](#)

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	48.0	7	29.2	14.0	0	0.0	0.0
PHI	24	48.0	5	20.8	10.0	0	0.0	0.0
CHI1	2	4.0	1	50.0	2.0	0	0.0	0.0
Total	50	100.0	13	26.0	26.0	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 [i](#)



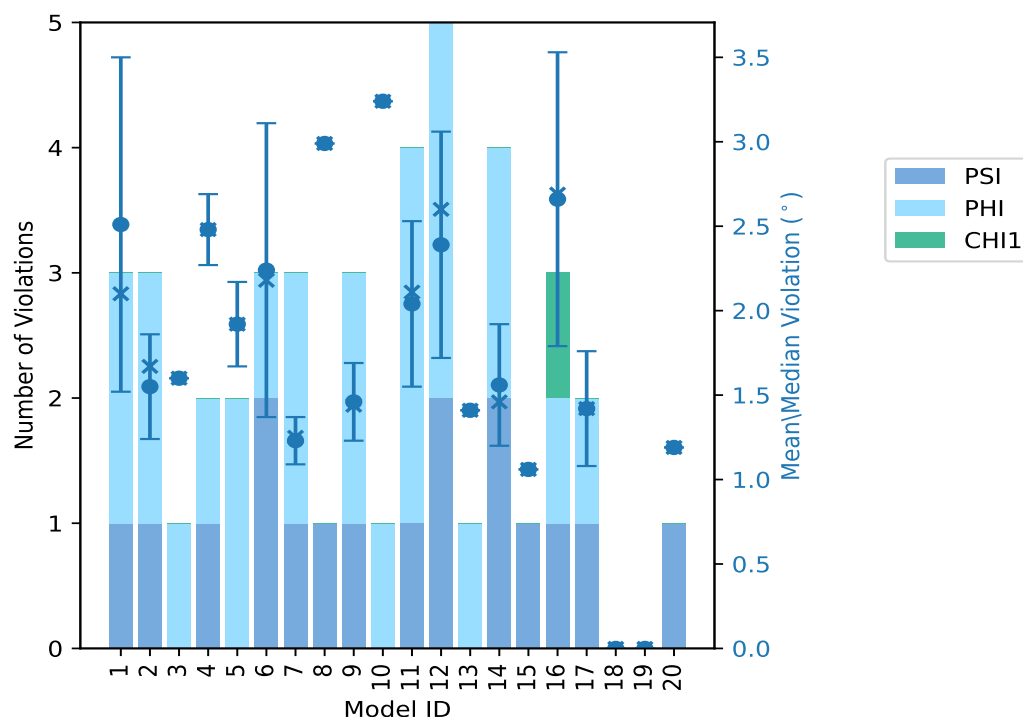
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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	1	2	0	3	2.51	3.88	0.99	2.1
2	1	2	0	3	1.55	1.86	0.31	1.67
3	0	1	0	1	1.6	1.6	0.0	1.6
4	1	1	0	2	2.48	2.69	0.21	2.48
5	0	2	0	2	1.92	2.16	0.25	1.92
6	2	1	0	3	2.24	3.34	0.87	2.18
7	1	2	0	3	1.23	1.39	0.14	1.25
8	1	0	0	1	2.99	2.99	0.0	2.99
9	1	2	0	3	1.46	1.75	0.23	1.44
10	0	1	0	1	3.24	3.24	0.0	3.24
11	1	3	0	4	2.04	2.59	0.49	2.11
12	2	3	0	5	2.39	3.02	0.67	2.6
13	0	1	0	1	1.41	1.41	0.0	1.41
14	2	2	0	4	1.56	2.12	0.36	1.46
15	1	0	0	1	1.06	1.06	0.0	1.06
16	1	1	1	3	2.66	3.72	0.87	2.69
17	1	1	0	2	1.42	1.76	0.34	1.42
18	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
20	1	0	0	1	1.19	1.19	0.0	1.19

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

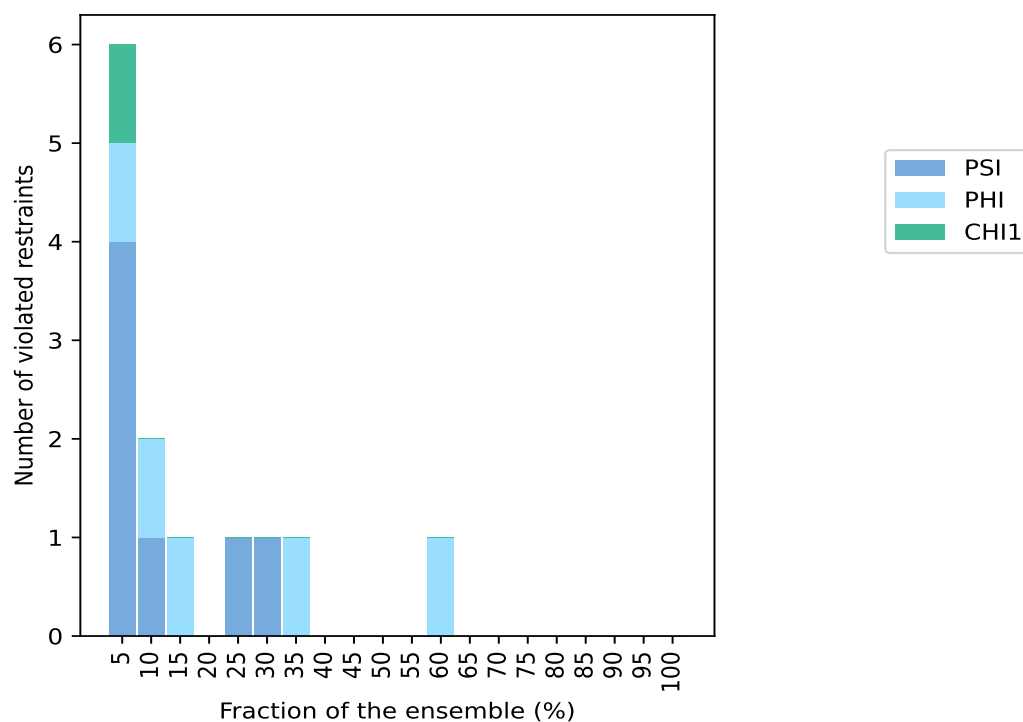
Continued on next page...

Continued from previous page...

Number of violated restraints				Fraction of the ensemble	
PSI	PHI	CHI1	Total	Count ¹	%
0	1	0	1	12	60.0
0	0	0	0	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 [i](#)

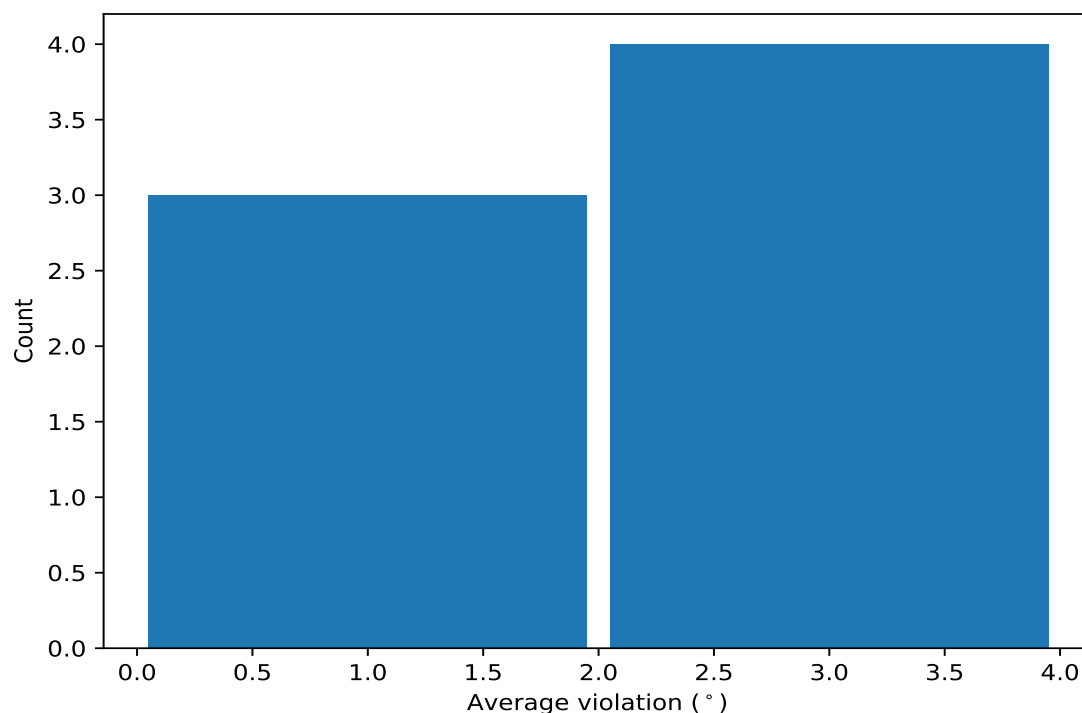


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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 [i](#)

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.

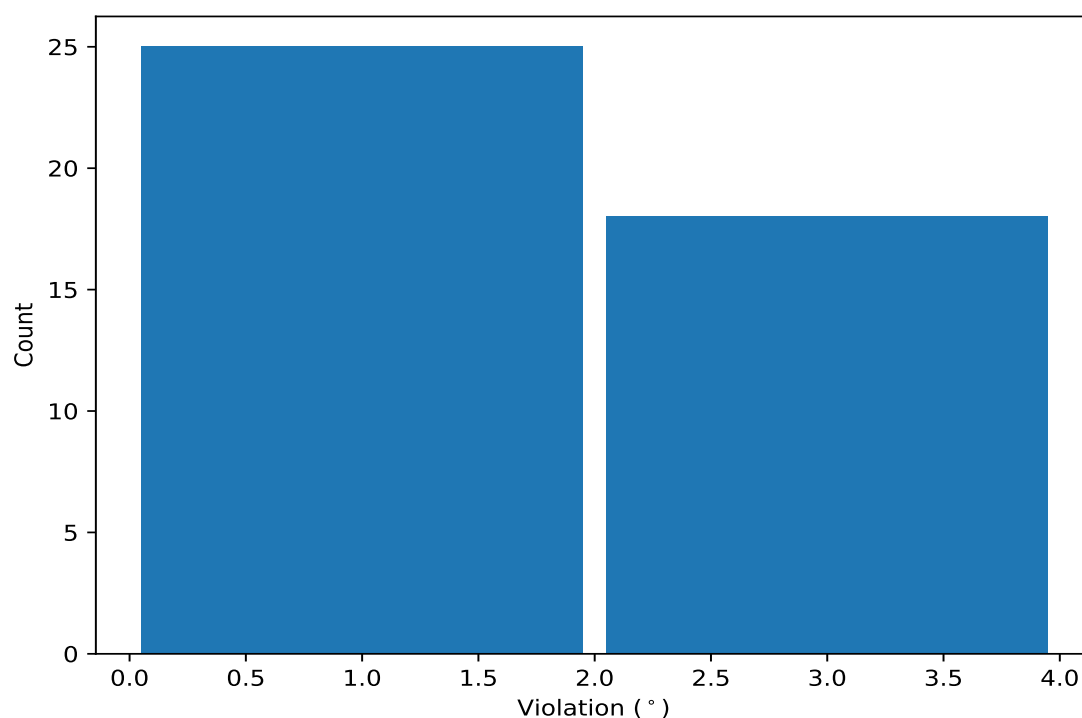
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,14)	1:38:A:SER:C	1:39:A:LYS:N	1:39:A:LYS:CA	1:39:A:LYS:C	12	1.67	0.54	1.48
(1,48)	1:57:A:LEU:C	1:58:A:LYS:N	1:58:A:LYS:CA	1:58:A:LYS:C	7	2.09	0.71	2.12
(1,43)	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	1:55:A:SER:N	6	2.01	0.52	1.81
(1,47)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:LYS:N	5	1.73	0.43	1.59
(1,24)	1:44:A:PRO:C	1:45:A:ALA:N	1:45:A:ALA:CA	1:45:A:ALA:C	3	1.97	0.65	2.1
(1,38)	1:51:A:GLU:C	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	2	2.92	0.33	2.92
(1,3)	1:31:A:PRO:N	1:31:A:PRO:CA	1:31:A:PRO:C	1:32:A:PHE:N	2	2.1	0.9	2.1

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

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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 [i](#)

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 (°)
(1,11)	1:36:A:GLU:N	1:36:A:GLU:CA	1:36:A:GLU:C	1:37:A:CYS:N	1	3.88
(1,49)	1:37:A:CYS:N	1:37:A:CYS:CA	1:37:A:CYS:CB	1:37:A:CYS:SG	16	3.72
(1,48)	1:57:A:LEU:C	1:58:A:LYS:N	1:58:A:LYS:CA	1:58:A:LYS:C	6	3.34
(1,38)	1:51:A:GLU:C	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	10	3.24
(1,43)	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	1:55:A:SER:N	12	3.02
(1,3)	1:31:A:PRO:N	1:31:A:PRO:CA	1:31:A:PRO:C	1:32:A:PHE:N	8	2.99
(1,14)	1:38:A:SER:C	1:39:A:LYS:N	1:39:A:LYS:CA	1:39:A:LYS:C	12	2.75
(1,24)	1:44:A:PRO:C	1:45:A:ALA:N	1:45:A:ALA:CA	1:45:A:ALA:C	4	2.69
(1,14)	1:38:A:SER:C	1:39:A:LYS:N	1:39:A:LYS:CA	1:39:A:LYS:C	16	2.69
(1,48)	1:57:A:LEU:C	1:58:A:LYS:N	1:58:A:LYS:CA	1:58:A:LYS:C	12	2.6