wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2KQB
BMRB ID	:	16596
Title	:	First PBZ domain of human APLF protein
Authors	:	Neuhaus, D.; Eustermann, S.; Brockmann, C.; Yang, J.
Deposited on	:	2009-11-04

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

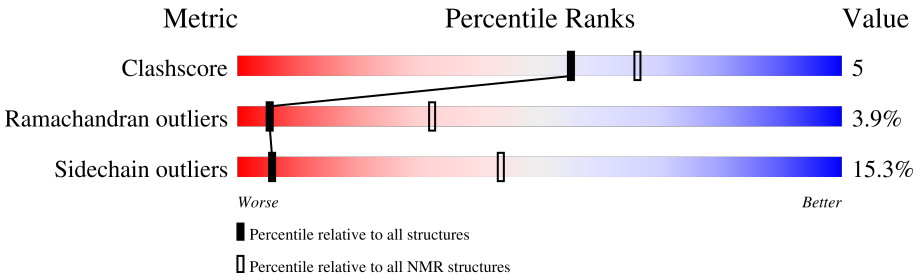
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 83%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	89	27% 8% 27% 38%

2 Ensemble composition and analysis

This entry contains 25 models. Model 17 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:374-A:404 (31)	0.38	17

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 3 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 11, 12, 19, 20, 21, 24, 25
2	6, 8, 9, 14, 15, 16, 17, 18, 22
3	2, 5, 7
Single-model clusters	10; 13; 23

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 792 atoms, of which 375 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Aprataxin and PNK-like factor.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	55	791	252	375	76	85	3	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	363	GLY	-	expression tag	UNP Q8IW19
A	364	PRO	-	expression tag	UNP Q8IW19
A	365	LEU	-	expression tag	UNP Q8IW19
A	366	GLY	-	expression tag	UNP Q8IW19
A	367	SER	-	expression tag	UNP Q8IW19

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

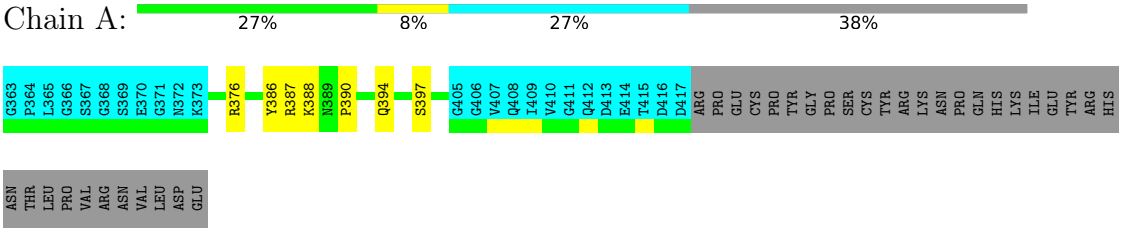
Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	1	1	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

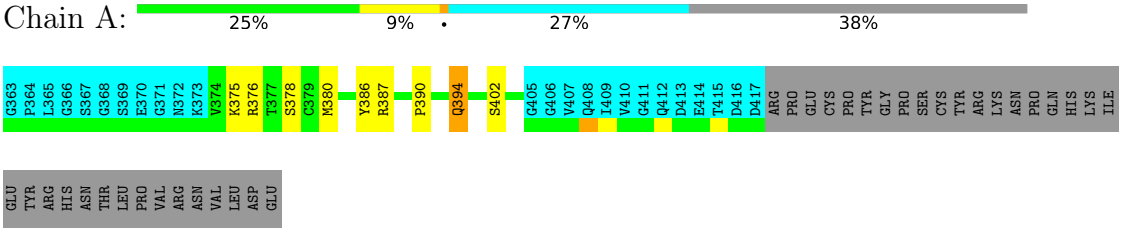
• Molecule 1: Aprataxin and PNK-like factor



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

The representative model is number 17. Colouring as in section 4.1 above.

• Molecule 1: Aprataxin and PNK-like factor



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 25 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
XPLOR-NIH	structure solution	
XPLOR-NIH	refinement	

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	937
Number of shifts mapped to atoms	562
Number of unparsed shifts	0
Number of shifts with mapping errors	375
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

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	255	229	228	3±1
All	All	6400	5725	5700	64

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 5.

5 of 17 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:384:ASN:O	1:A:386:TYR:N	0.49	2.45	5	6
1:A:376:ARG:CB	1:A:397:SER:OG	0.49	2.61	23	10
1:A:386:TYR:CD1	1:A:387:ARG:N	0.48	2.81	19	20
1:A:386:TYR:OH	1:A:387:ARG:NH1	0.47	2.48	4	1
1:A:378:SER:OG	1:A:404:TYR:CE1	0.46	2.65	4	2

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	31/89 (35%)	27±2 (86±6%)	3±1 (10±5%)	1±1 (4±2%)	5 32
All	All	775/2225 (35%)	668 (86%)	77 (10%)	30 (4%)	5 32

5 of 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	390	PRO	13
1	A	385	CYS	6
1	A	382	GLY	5
1	A	379	CYS	2
1	A	391	VAL	2

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	28/78 (36%)	24±1 (85±4%)	4±1 (15±4%)	6 43
All	All	700/1950 (36%)	593 (85%)	107 (15%)	6 43

5 of 12 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	394	GLN	22
1	A	387	ARG	16
1	A	376	ARG	16
1	A	388	LYS	15
1	A	397	SER	9

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

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

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 84% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

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	937
Number of shifts mapped to atoms	562
Number of unparsed shifts	0
Number of shifts with mapping errors	375
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 375) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	418	ARG	H	7.891	0.020	1
1	A	418	ARG	HA	4.413	0.020	1
1	A	418	ARG	HB2	1.689	0.020	2
1	A	418	ARG	HB3	1.667	0.020	2
1	A	418	ARG	HD2	3.276	0.020	2
1	A	418	ARG	HD3	2.796	0.020	2
1	A	418	ARG	HG2	1.796	0.020	2
1	A	418	ARG	HG3	1.672	0.020	2
1	A	418	ARG	CA	55.001	0.100	1
1	A	418	ARG	CB	30.612	0.100	1
1	A	418	ARG	CD	44.073	0.100	1
1	A	418	ARG	CG	26.348	0.100	1
1	A	418	ARG	N	121.518	0.100	1
1	A	419	PRO	HA	4.535	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	419	PRO	HB2	2.34	0.020	2
1	A	419	PRO	HB3	1.982	0.020	2
1	A	419	PRO	HD2	3.754	0.020	2
1	A	419	PRO	HD3	3.687	0.020	2
1	A	419	PRO	HG2	1.853	0.020	1
1	A	419	PRO	HG3	1.853	0.020	1
1	A	419	PRO	CA	61.998	0.100	1
1	A	419	PRO	CB	31.823	0.100	1
1	A	419	PRO	CD	50.164	0.100	1
1	A	419	PRO	CG	27.106	0.100	1
1	A	420	GLU	H	8.597	0.020	1
1	A	420	GLU	HA	4.225	0.020	1
1	A	420	GLU	HB2	1.882	0.020	1
1	A	420	GLU	HB3	1.882	0.020	1
1	A	420	GLU	HG2	2.233	0.020	2
1	A	420	GLU	HG3	2.191	0.020	2
1	A	420	GLU	CA	55.891	0.100	1
1	A	420	GLU	CB	30.367	0.100	1
1	A	420	GLU	CG	36.356	0.100	1
1	A	420	GLU	N	120.636	0.100	1
1	A	421	CYS	H	8.303	0.020	1
1	A	421	CYS	HA	4.099	0.020	1
1	A	421	CYS	HB2	2.406	0.020	2
1	A	421	CYS	HB3	1.789	0.020	2
1	A	421	CYS	CA	57.311	0.100	1
1	A	421	CYS	CB	29.319	0.100	1
1	A	421	CYS	N	127.139	0.100	1
1	A	422	PRO	HA	4.355	0.020	1
1	A	422	PRO	HB2	2.146	0.020	2
1	A	422	PRO	HB3	1.521	0.020	2
1	A	422	PRO	HD2	3.571	0.020	2
1	A	422	PRO	HD3	3.452	0.020	2
1	A	422	PRO	HG2	1.768	0.020	2
1	A	422	PRO	HG3	1.203	0.020	2
1	A	422	PRO	CA	64.044	0.100	1
1	A	422	PRO	CB	32.088	0.100	1
1	A	422	PRO	CD	51.58	0.100	1
1	A	422	PRO	CG	26.295	0.100	1
1	A	423	TYR	H	8.64	0.020	1
1	A	423	TYR	HA	4.545	0.020	1
1	A	423	TYR	HB2	3.145	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	423	TYR	HB3	2.967	0.020	2
1	A	423	TYR	HD1	7.177	0.020	3
1	A	423	TYR	HD2	7.177	0.020	3
1	A	423	TYR	HE1	6.768	0.020	3
1	A	423	TYR	HE2	6.768	0.020	3
1	A	423	TYR	CA	58.527	0.100	1
1	A	423	TYR	CB	37.549	0.100	1
1	A	423	TYR	CD1	133.004	0.100	3
1	A	423	TYR	CD2	133.004	0.100	3
1	A	423	TYR	CE1	118.119	0.100	3
1	A	423	TYR	CE2	118.119	0.100	3
1	A	423	TYR	N	119.569	0.100	1
1	A	424	GLY	H	7.606	0.020	1
1	A	424	GLY	HA2	4.021	0.020	2
1	A	424	GLY	HA3	4.379	0.020	2
1	A	424	GLY	CA	45.77	0.100	1
1	A	424	GLY	N	107.733	0.100	1
1	A	425	PRO	HA	4.56	0.020	1
1	A	425	PRO	HB2	2.459	0.020	1
1	A	425	PRO	HB3	2.459	0.020	1
1	A	425	PRO	HD2	3.977	0.020	2
1	A	425	PRO	HD3	3.763	0.020	2
1	A	425	PRO	HG2	2.109	0.020	1
1	A	425	PRO	HG3	2.109	0.020	1
1	A	425	PRO	CA	64.402	0.100	1
1	A	425	PRO	CB	32.223	0.100	1
1	A	425	PRO	CD	50.654	0.100	1
1	A	425	PRO	CG	27.201	0.100	1
1	A	426	SER	H	8.072	0.020	1
1	A	426	SER	HA	4.566	0.020	1
1	A	426	SER	HB2	4.038	0.020	1
1	A	426	SER	HB3	4.038	0.020	1
1	A	426	SER	CA	57.738	0.100	1
1	A	426	SER	CB	63.162	0.100	1
1	A	426	SER	N	112.851	0.100	1
1	A	427	CYS	H	7.606	0.020	1
1	A	427	CYS	HA	3.724	0.020	1
1	A	427	CYS	HB2	3.338	0.020	2
1	A	427	CYS	HB3	3.058	0.020	2
1	A	427	CYS	CA	61.712	0.100	1
1	A	427	CYS	CB	29.798	0.100	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	427	CYS	N	123.514	0.100	1
1	A	428	TYR	H	7.686	0.020	1
1	A	428	TYR	HA	4.782	0.020	1
1	A	428	TYR	HB2	3.128	0.020	2
1	A	428	TYR	HB3	2.989	0.020	2
1	A	428	TYR	HD1	7.071	0.020	3
1	A	428	TYR	HD2	7.071	0.020	3
1	A	428	TYR	HE1	6.737	0.020	3
1	A	428	TYR	HE2	6.737	0.020	3
1	A	428	TYR	CA	56.505	0.100	1
1	A	428	TYR	CB	38.153	0.100	1
1	A	428	TYR	CD1	133.56	0.100	3
1	A	428	TYR	CD2	133.56	0.100	3
1	A	428	TYR	CE1	118.267	0.100	3
1	A	428	TYR	CE2	118.267	0.100	3
1	A	428	TYR	N	126.466	0.100	1
1	A	429	ARG	H	7.969	0.020	1
1	A	429	ARG	HA	4.012	0.020	1
1	A	429	ARG	HB2	1.508	0.020	2
1	A	429	ARG	HB3	1.203	0.020	2
1	A	429	ARG	HD2	2.466	0.020	2
1	A	429	ARG	HD3	2.373	0.020	2
1	A	429	ARG	HG2	1.194	0.020	2
1	A	429	ARG	HG3	1.009	0.020	2
1	A	429	ARG	CA	57.177	0.100	1
1	A	429	ARG	CB	29.875	0.100	1
1	A	429	ARG	CD	42.234	0.100	1
1	A	429	ARG	CG	26.779	0.100	1
1	A	429	ARG	N	123.918	0.100	1
1	A	432	PRO	HA	4.254	0.020	1
1	A	432	PRO	HB2	2.47	0.020	1
1	A	432	PRO	HB3	2.47	0.020	1
1	A	432	PRO	HD2	4.107	0.020	2
1	A	432	PRO	HD3	3.945	0.020	2
1	A	432	PRO	HG2	2.219	0.020	2
1	A	432	PRO	HG3	2.104	0.020	2
1	A	432	PRO	CA	65.569	0.100	1
1	A	432	PRO	CB	32.244	0.100	1
1	A	432	PRO	CD	51.419	0.100	1
1	A	432	PRO	CG	27.639	0.100	1
1	A	433	GLN	H	8.407	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	433	GLN	HA	4.107	0.020	1
1	A	433	GLN	HB2	2.218	0.020	2
1	A	433	GLN	HB3	2.118	0.020	2
1	A	433	GLN	HE21	7.801	0.020	1
1	A	433	GLN	HE22	6.897	0.020	1
1	A	433	GLN	HG2	2.499	0.020	1
1	A	433	GLN	HG3	2.499	0.020	1
1	A	433	GLN	CA	58.51	0.100	1
1	A	433	GLN	CB	27.706	0.100	1
1	A	433	GLN	CG	33.702	0.100	1
1	A	433	GLN	N	116.801	0.100	1
1	A	433	GLN	NE2	112.339	0.100	1
1	A	434	HIS	H	8.002	0.020	1
1	A	434	HIS	HA	4.575	0.020	1
1	A	434	HIS	HB2	3.398	0.020	2
1	A	434	HIS	HB3	3.389	0.020	2
1	A	434	HIS	HD2	6.961	0.020	1
1	A	434	HIS	HE1	7.66	0.020	1
1	A	434	HIS	CA	60.168	0.100	1
1	A	434	HIS	CB	28.212	0.100	1
1	A	434	HIS	CD2	127.471	0.100	1
1	A	434	HIS	CE1	139.924	0.100	1
1	A	434	HIS	N	119.182	0.100	1
1	A	435	LYS	H	7.26	0.020	1
1	A	435	LYS	HA	4.166	0.020	1
1	A	435	LYS	HB2	2.028	0.020	2
1	A	435	LYS	HB3	1.889	0.020	2
1	A	435	LYS	HD2	1.614	0.020	1
1	A	435	LYS	HD3	1.614	0.020	1
1	A	435	LYS	HE2	2.899	0.020	1
1	A	435	LYS	HE3	2.899	0.020	1
1	A	435	LYS	HG2	1.586	0.020	2
1	A	435	LYS	HG3	1.288	0.020	2
1	A	435	LYS	CA	58.305	0.100	1
1	A	435	LYS	CB	32.328	0.100	1
1	A	435	LYS	CD	29.149	0.100	1
1	A	435	LYS	CE	41.856	0.100	1
1	A	435	LYS	CG	25.768	0.100	1
1	A	435	LYS	N	113.956	0.100	1
1	A	436	ILE	H	7.417	0.020	1
1	A	436	ILE	HA	3.996	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	436	ILE	HB	1.998	0.020	1
1	A	436	ILE	HD11	0.867	0.020	1
1	A	436	ILE	HD12	0.867	0.020	1
1	A	436	ILE	HD13	0.867	0.020	1
1	A	436	ILE	HG12	1.636	0.020	2
1	A	436	ILE	HG13	1.253	0.020	2
1	A	436	ILE	HG21	0.929	0.020	1
1	A	436	ILE	HG22	0.929	0.020	1
1	A	436	ILE	HG23	0.929	0.020	1
1	A	436	ILE	CA	62.746	0.100	1
1	A	436	ILE	CB	38.648	0.100	1
1	A	436	ILE	CD1	12.811	0.100	1
1	A	436	ILE	CG1	28.803	0.100	1
1	A	436	ILE	CG2	17.474	0.100	1
1	A	436	ILE	N	117.362	0.100	1
1	A	437	GLU	H	7.787	0.020	1
1	A	437	GLU	HA	3.881	0.020	1
1	A	437	GLU	HB2	1.997	0.020	2
1	A	437	GLU	HB3	1.729	0.020	2
1	A	437	GLU	HG2	2.349	0.020	2
1	A	437	GLU	HG3	1.965	0.020	2
1	A	437	GLU	CA	58.513	0.100	1
1	A	437	GLU	CB	31.109	0.100	1
1	A	437	GLU	CG	36.444	0.100	1
1	A	437	GLU	N	120.444	0.100	1
1	A	438	TYR	H	7.383	0.020	1
1	A	438	TYR	HA	4.882	0.020	1
1	A	438	TYR	HB2	2.409	0.020	2
1	A	438	TYR	HB3	2.062	0.020	2
1	A	438	TYR	HD1	6.905	0.020	3
1	A	438	TYR	HD2	6.905	0.020	3
1	A	438	TYR	HE1	6.907	0.020	3
1	A	438	TYR	HE2	6.907	0.020	3
1	A	438	TYR	CA	56.405	0.100	1
1	A	438	TYR	CB	41.759	0.100	1
1	A	438	TYR	CD1	133.671	0.100	3
1	A	438	TYR	CD2	133.671	0.100	3
1	A	438	TYR	CE1	117.854	0.100	3
1	A	438	TYR	CE2	117.854	0.100	3
1	A	438	TYR	N	112.626	0.100	1
1	A	439	ARG	H	8.474	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	439	ARG	HA	4.497	0.020	1
1	A	439	ARG	HB2	1.622	0.020	1
1	A	439	ARG	HB3	1.622	0.020	1
1	A	439	ARG	HD2	3.248	0.020	2
1	A	439	ARG	HD3	3.156	0.020	2
1	A	439	ARG	HG2	1.492	0.020	1
1	A	439	ARG	HG3	1.492	0.020	1
1	A	439	ARG	CA	55.405	0.100	1
1	A	439	ARG	CB	32.042	0.100	1
1	A	439	ARG	CD	43.742	0.100	1
1	A	439	ARG	CG	27.404	0.100	1
1	A	439	ARG	N	118.284	0.100	1
1	A	440	HIS	H	8.889	0.020	1
1	A	440	HIS	HA	4.807	0.020	1
1	A	440	HIS	HB2	3.37	0.020	2
1	A	440	HIS	HB3	2.889	0.020	2
1	A	440	HIS	HD2	7.338	0.020	1
1	A	440	HIS	HE1	7.216	0.020	1
1	A	440	HIS	CA	57.095	0.100	1
1	A	440	HIS	CB	30.316	0.100	1
1	A	440	HIS	CD2	127.643	0.100	1
1	A	440	HIS	CE1	137.437	0.100	1
1	A	440	HIS	N	121.568	0.100	1
1	A	441	ASN	H	8.876	0.020	1
1	A	441	ASN	HA	4.876	0.020	1
1	A	441	ASN	HB2	2.895	0.020	2
1	A	441	ASN	HB3	2.881	0.020	2
1	A	441	ASN	HD21	7.783	0.020	1
1	A	441	ASN	HD22	7.055	0.020	1
1	A	441	ASN	CA	53.387	0.100	1
1	A	441	ASN	CB	39.039	0.100	1
1	A	441	ASN	N	120.377	0.100	1
1	A	441	ASN	ND2	113.374	0.100	1
1	A	442	THR	H	8.264	0.020	1
1	A	442	THR	HA	4.372	0.020	1
1	A	442	THR	HB	4.237	0.020	1
1	A	442	THR	HG21	1.239	0.020	1
1	A	442	THR	HG22	1.239	0.020	1
1	A	442	THR	HG23	1.239	0.020	1
1	A	442	THR	CA	61.787	0.100	1
1	A	442	THR	CB	69.844	0.100	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	442	THR	CG2	21.868	0.100	1
1	A	442	THR	N	114.401	0.100	1
1	A	443	LEU	H	8.323	0.020	1
1	A	443	LEU	HA	4.683	0.020	1
1	A	443	LEU	HB2	1.672	0.020	2
1	A	443	LEU	HB3	1.615	0.020	2
1	A	443	LEU	HD11	0.996	0.020	2
1	A	443	LEU	HD12	0.996	0.020	2
1	A	443	LEU	HD13	0.996	0.020	2
1	A	443	LEU	HD21	0.97	0.020	2
1	A	443	LEU	HD22	0.97	0.020	2
1	A	443	LEU	HD23	0.97	0.020	2
1	A	443	LEU	HG	1.718	0.020	1
1	A	443	LEU	CA	53.096	0.100	1
1	A	443	LEU	CB	41.921	0.100	1
1	A	443	LEU	CD1	25.296	0.100	2
1	A	443	LEU	CD2	23.591	0.100	2
1	A	443	LEU	CG	26.968	0.100	1
1	A	443	LEU	N	125.734	0.100	1
1	A	444	PRO	HA	4.5	0.020	1
1	A	444	PRO	HB2	2.314	0.020	2
1	A	444	PRO	HB3	1.916	0.020	2
1	A	444	PRO	HD2	3.905	0.020	2
1	A	444	PRO	HD3	3.686	0.020	2
1	A	444	PRO	HG2	2.061	0.020	1
1	A	444	PRO	HG3	2.061	0.020	1
1	A	444	PRO	CA	63.018	0.100	1
1	A	444	PRO	CB	32.036	0.100	1
1	A	444	PRO	CD	50.676	0.100	1
1	A	444	PRO	CG	27.427	0.100	1
1	A	445	VAL	H	8.244	0.020	1
1	A	445	VAL	HA	4.106	0.020	1
1	A	445	VAL	HB	2.079	0.020	1
1	A	445	VAL	HG11	0.997	0.020	2
1	A	445	VAL	HG12	0.997	0.020	2
1	A	445	VAL	HG13	0.997	0.020	2
1	A	445	VAL	HG21	0.999	0.020	2
1	A	445	VAL	HG22	0.999	0.020	2
1	A	445	VAL	HG23	0.999	0.020	2
1	A	445	VAL	CA	62.328	0.100	1
1	A	445	VAL	CB	32.784	0.100	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	445	VAL	CG1	20.743	0.100	2
1	A	445	VAL	CG2	20.759	0.100	2
1	A	445	VAL	N	120.697	0.100	1
1	A	446	ARG	H	8.419	0.020	1
1	A	446	ARG	HA	4.41	0.020	1
1	A	446	ARG	HB2	1.857	0.020	2
1	A	446	ARG	HB3	1.78	0.020	2
1	A	446	ARG	HD2	3.22	0.020	1
1	A	446	ARG	HD3	3.22	0.020	1
1	A	446	ARG	HG2	1.668	0.020	2
1	A	446	ARG	HG3	1.611	0.020	2
1	A	446	ARG	CA	55.85	0.100	1
1	A	446	ARG	CB	31.161	0.100	1
1	A	446	ARG	CD	43.434	0.100	1
1	A	446	ARG	CG	27.154	0.100	1
1	A	446	ARG	N	124.912	0.100	1
1	A	447	ASN	H	8.604	0.020	1
1	A	447	ASN	HA	4.777	0.020	1
1	A	447	ASN	HB2	2.872	0.020	2
1	A	447	ASN	HB3	2.764	0.020	2
1	A	447	ASN	HD21	7.646	0.020	1
1	A	447	ASN	HD22	6.924	0.020	1
1	A	447	ASN	CA	53.14	0.100	1
1	A	447	ASN	CB	39.022	0.100	1
1	A	447	ASN	N	121.258	0.100	1
1	A	447	ASN	ND2	112.844	0.100	1
1	A	448	VAL	H	8.187	0.020	1
1	A	448	VAL	HA	4.142	0.020	1
1	A	448	VAL	HB	2.14	0.020	1
1	A	448	VAL	HG11	0.956	0.020	2
1	A	448	VAL	HG12	0.956	0.020	2
1	A	448	VAL	HG13	0.956	0.020	2
1	A	448	VAL	HG21	0.957	0.020	2
1	A	448	VAL	HG22	0.957	0.020	2
1	A	448	VAL	HG23	0.957	0.020	2
1	A	448	VAL	CA	62.595	0.100	1
1	A	448	VAL	CB	32.681	0.100	1
1	A	448	VAL	CG1	21.278	0.100	2
1	A	448	VAL	CG2	20.388	0.100	2
1	A	448	VAL	N	120.745	0.100	1
1	A	449	LEU	H	8.311	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	449	LEU	HA	4.416	0.020	1
1	A	449	LEU	HB2	1.627	0.020	1
1	A	449	LEU	HB3	1.627	0.020	1
1	A	449	LEU	HD11	0.9	0.020	1
1	A	449	LEU	HD12	0.9	0.020	1
1	A	449	LEU	HD13	0.9	0.020	1
1	A	449	LEU	HD21	0.9	0.020	1
1	A	449	LEU	HD22	0.9	0.020	1
1	A	449	LEU	HD23	0.9	0.020	1
1	A	449	LEU	HG	1.644	0.020	1
1	A	449	LEU	CA	55.141	0.100	1
1	A	449	LEU	CB	42.344	0.100	1
1	A	449	LEU	CD1	24.933	0.100	2
1	A	449	LEU	CD2	23.39	0.100	2
1	A	449	LEU	CG	27.115	0.100	1
1	A	449	LEU	N	124.673	0.100	1
1	A	450	ASP	H	8.239	0.020	1
1	A	450	ASP	HA	4.665	0.020	1
1	A	450	ASP	HB2	2.781	0.020	2
1	A	450	ASP	HB3	2.62	0.020	2
1	A	450	ASP	CA	54.364	0.100	1
1	A	450	ASP	CB	41.126	0.100	1
1	A	450	ASP	N	121.582	0.100	1
1	A	451	GLU	H	7.813	0.020	1
1	A	451	GLU	HA	4.165	0.020	1
1	A	451	GLU	HB2	2.067	0.020	2
1	A	451	GLU	HB3	1.921	0.020	2
1	A	451	GLU	HG2	2.232	0.020	1
1	A	451	GLU	HG3	2.232	0.020	1
1	A	451	GLU	CA	57.917	0.100	1
1	A	451	GLU	CB	31.405	0.100	1
1	A	451	GLU	CG	36.595	0.100	1
1	A	451	GLU	N	125.775	0.100	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
$^{13}C_{\alpha}$	86	-0.19 ± 0.26	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	77	0.25 ± 0.22	None needed (< 0.5 ppm)

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C'$	0	—	None (insufficient data)
^{15}N	78	-0.77 ± 0.43	None needed (imprecise)

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 83%, i.e. 344 atoms were assigned a chemical shift out of a possible 413. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	122/153 (80%)	62/62 (100%)	31/62 (50%)	29/29 (100%)
Sidechain	166/191 (87%)	112/122 (92%)	51/58 (88%)	3/11 (27%)
Aromatic	56/69 (81%)	28/34 (82%)	28/31 (90%)	0/4 (0%)
Overall	344/413 (83%)	202/218 (93%)	110/151 (73%)	32/44 (73%)

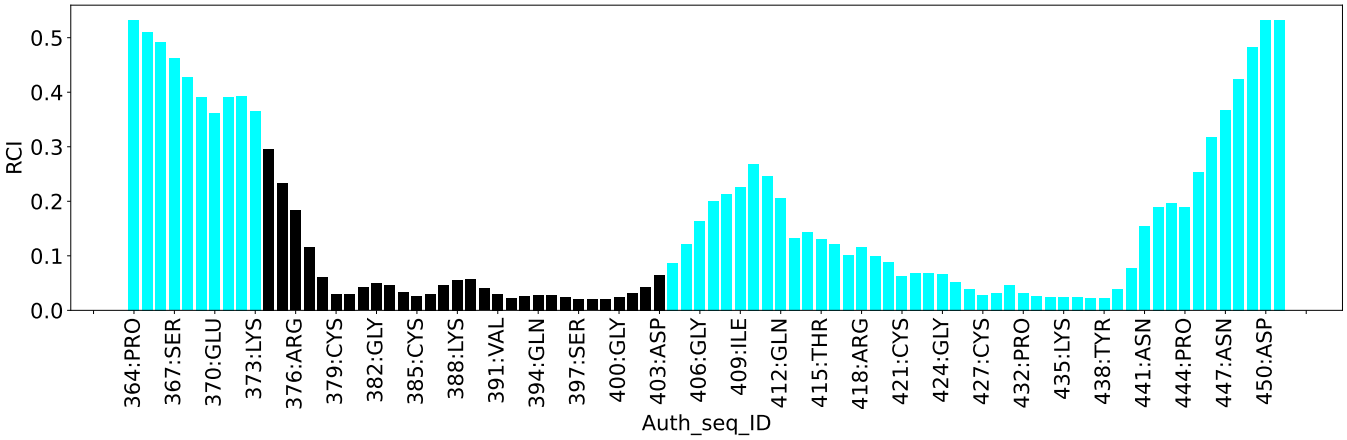
7.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots

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

Random coil index (RCI) for chain A:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
364:PRO
367:SER
370:GLU
373:LYS
376:ARG
379:CYS
382:GLY
385:CYS
388:LYS
391:VAL
394:GLN
397:SER
400:GLY
403:ASP
406:GLY
409:ILE
412:GLN
415:THR
418:ARG
421:CYS
424:GLY
427:CYS
432:PRO
435:LYS
438:TYR
441:ASN
444:PRO
447:ASN
450:ASP
Auth_seq_ID

8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	721
Intra-residue (|i-j|=0)	151
Sequential (|i-j|=1)	269
Medium range (|i-j|>1 and |i-j|<5)	163
Long range (|i-j|≥5)	133
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	5
Total dihedral-angle restraints	36
Number of unmapped restraints	8
Number of restraints per residue	8.5
Number of long range restraints per residue[1]	1.6

[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)	10.6	0.2
0.2-0.5 (Medium)	1.3	0.5
>0.5 (Large)	0.2	0.56

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)	4.7	9.9
10.0-20.0 (Medium)	1.4	19.9
>20.0 (Large)	0.0	21.7

9 Distance violation analysis (i)

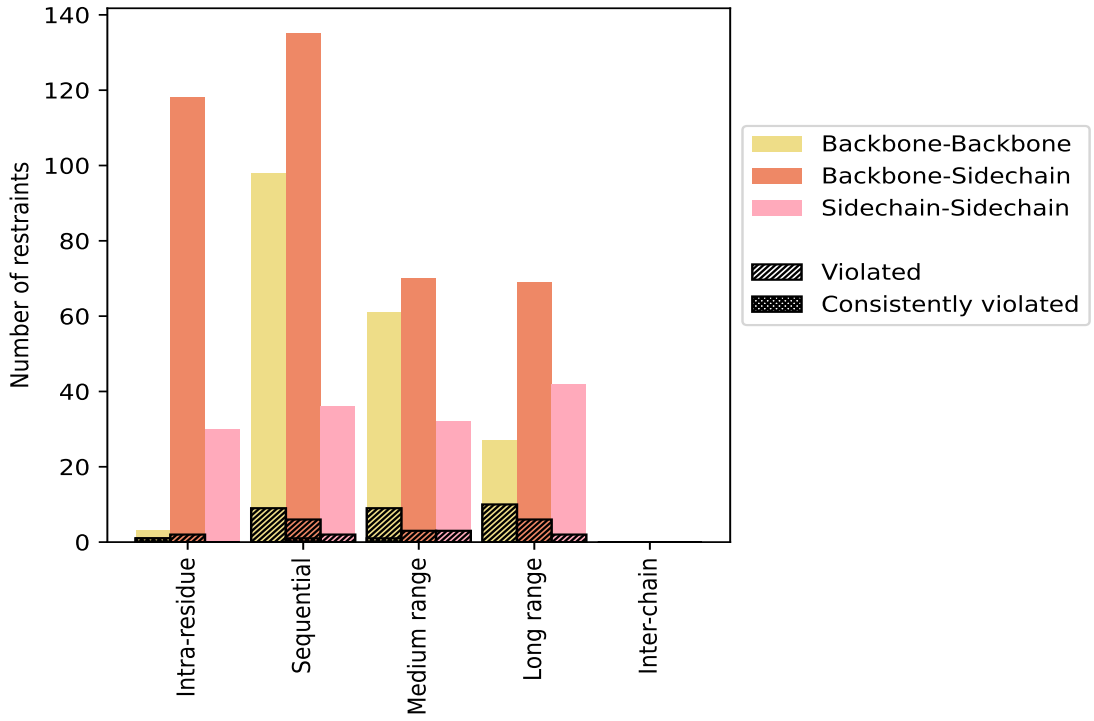
9.1 Summary of distance violations (i)

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)	151	20.9	3	2.0	0.4	1	0.7	0.1
Backbone-Backbone	3	0.4	1	33.3	0.1	1	33.3	0.1
Backbone-Sidechain	118	16.4	2	1.7	0.3	0	0.0	0.0
Sidechain-Sidechain	30	4.2	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	269	37.3	17	6.3	2.4	1	0.4	0.1
Backbone-Backbone	98	13.6	9	9.2	1.2	0	0.0	0.0
Backbone-Sidechain	135	18.7	6	4.4	0.8	1	0.7	0.1
Sidechain-Sidechain	36	5.0	2	5.6	0.3	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	163	22.6	15	9.2	2.1	1	0.6	0.1
Backbone-Backbone	61	8.5	9	14.8	1.2	1	1.6	0.1
Backbone-Sidechain	70	9.7	3	4.3	0.4	0	0.0	0.0
Sidechain-Sidechain	32	4.4	3	9.4	0.4	0	0.0	0.0
Long range (|i-j|≥5)	133	18.4	18	13.5	2.5	0	0.0	0.0
Backbone-Backbone	27	3.7	10	37.0	1.4	0	0.0	0.0
Backbone-Sidechain	69	9.6	6	8.7	0.8	0	0.0	0.0
Sidechain-Sidechain	37	5.1	2	5.4	0.3	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	5	0.7	0	0.0	0.0	0	0.0	0.0
Total	721	100.0	53	7.4	7.4	3	0.4	0.4
Backbone-Backbone	189	26.2	29	15.3	4.0	2	1.1	0.3
Backbone-Sidechain	392	54.4	17	4.3	2.4	1	0.3	0.1
Sidechain-Sidechain	140	19.4	7	5.0	1.0	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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	2	3	4	5	0	14	0.16	0.22	0.03	0.16
2	2	2	5	4	0	13	0.15	0.22	0.03	0.14
3	3	4	4	6	0	17	0.14	0.24	0.04	0.14
4	1	2	5	3	0	11	0.15	0.27	0.04	0.13
5	1	3	5	2	0	11	0.14	0.17	0.02	0.13
6	2	3	2	3	0	10	0.15	0.27	0.04	0.14
7	1	3	5	3	0	12	0.16	0.25	0.03	0.15
8	1	3	3	4	0	11	0.17	0.51	0.11	0.13
9	1	9	2	4	0	16	0.15	0.22	0.03	0.15
10	2	4	2	6	0	14	0.15	0.18	0.02	0.15
11	1	1	6	4	0	12	0.17	0.3	0.05	0.16

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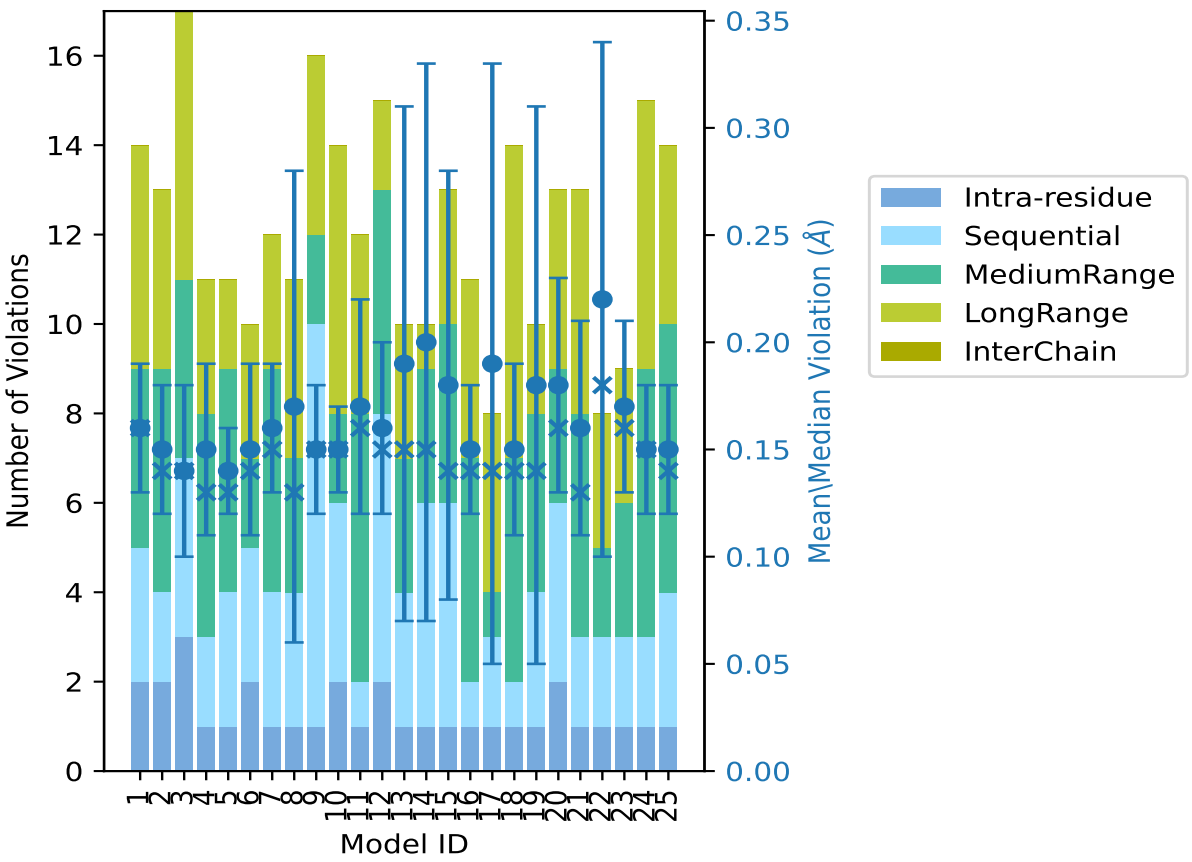
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	2	6	5	2	0	15	0.16	0.26	0.04	0.15
13	1	3	3	3	0	10	0.19	0.53	0.12	0.15
14	1	5	3	1	0	10	0.2	0.56	0.13	0.15
15	1	5	4	3	0	13	0.18	0.5	0.1	0.14
16	1	1	5	4	0	11	0.15	0.2	0.03	0.14
17	1	2	1	4	0	8	0.19	0.56	0.14	0.14
18	1	1	5	7	0	14	0.15	0.24	0.04	0.14
19	1	3	4	2	0	10	0.18	0.55	0.13	0.14
20	2	4	3	4	0	13	0.18	0.33	0.05	0.16
21	1	2	5	5	0	13	0.16	0.29	0.05	0.13
22	1	2	2	3	0	8	0.22	0.52	0.12	0.18
23	1	2	3	3	0	9	0.17	0.23	0.04	0.16
24	1	2	6	6	0	15	0.15	0.22	0.03	0.15
25	1	3	6	4	0	14	0.15	0.21	0.03	0.14

[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

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, 663(IR:148, SQ:252, MR:148, LR:115, 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]	%
0	4	4	7	0	15	1	4.0
1	4	2	0	0	7	2	8.0
0	1	0	2	0	3	3	12.0
0	3	1	1	0	5	4	16.0
0	1	0	2	0	3	5	20.0
1	1	3	2	0	7	6	24.0

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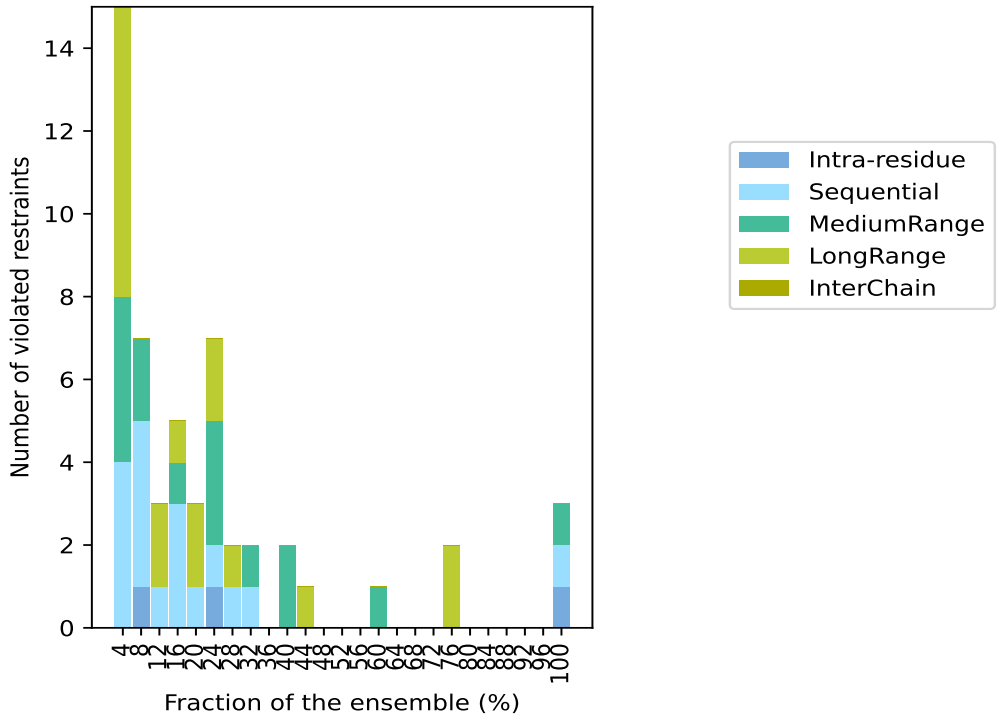
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	1	0	1	0	2	7	28.0
0	1	1	0	0	2	8	32.0
0	0	0	0	0	0	9	36.0
0	0	2	0	0	2	10	40.0
0	0	0	1	0	1	11	44.0
0	0	0	0	0	0	12	48.0
0	0	0	0	0	0	13	52.0
0	0	0	0	0	0	14	56.0
0	0	1	0	0	1	15	60.0
0	0	0	0	0	0	16	64.0
0	0	0	0	0	0	17	68.0
0	0	0	0	0	0	18	72.0
0	0	0	2	0	2	19	76.0
0	0	0	0	0	0	20	80.0
0	0	0	0	0	0	21	84.0
0	0	0	0	0	0	22	88.0
0	0	0	0	0	0	23	92.0
0	0	0	0	0	0	24	96.0
1	1	1	0	0	3	25	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

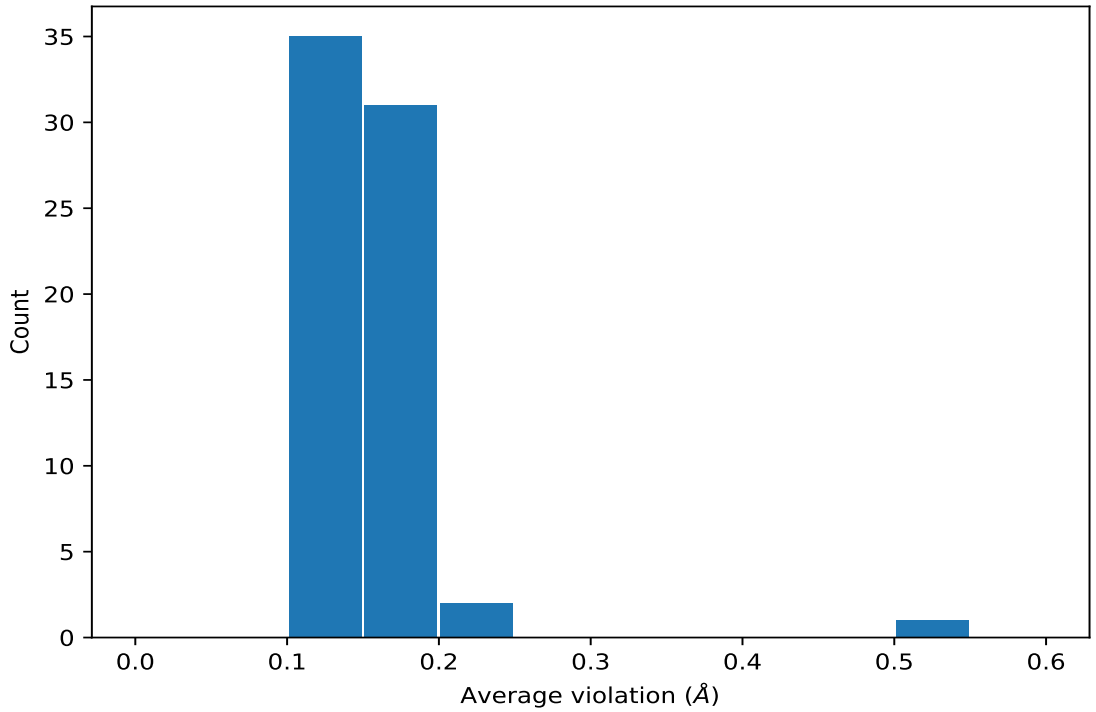
9.3.1 Bar graph : Distance violation statistics for the ensemble



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.

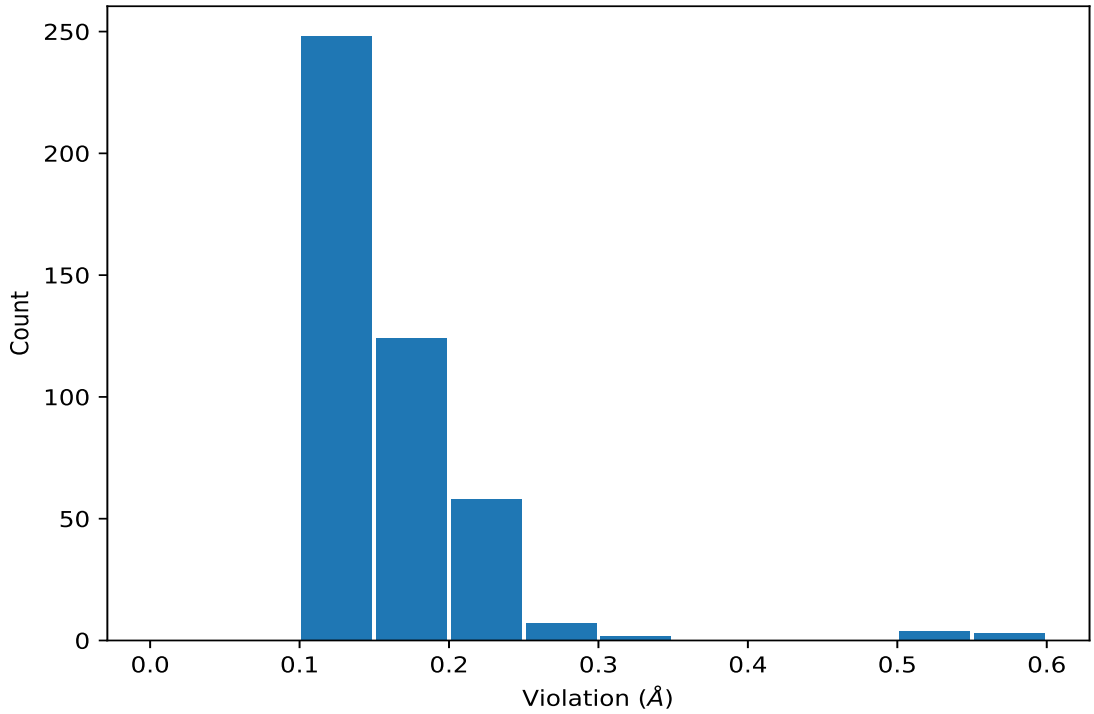
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,530)	1:A:401:ASP:H	1:A:403:ASP:H	25	0.19	0.05	0.2
(1,96)	1:A:376:ARG:HA	1:A:377:THR:HB	25	0.17	0.03	0.16
(1,86)	1:A:376:ARG:H	1:A:376:ARG:HA	25	0.17	0.02	0.17
(1,85)	1:A:375:LYS:HA	1:A:403:ASP:H	19	0.16	0.05	0.14
(1,182)	1:A:379:CYS:H	1:A:397:SER:HA	19	0.15	0.03	0.15
(1,365)	1:A:391:VAL:H	1:A:394:GLN:H	15	0.14	0.02	0.13
(1,503)	1:A:398:HIS:HA	1:A:405:GLY:H	11	0.15	0.02	0.15
(1,371)	1:A:391:VAL:HB	1:A:394:GLN:HE22	10	0.14	0.02	0.14
(1,400)	1:A:392:HIS:HB2	1:A:394:GLN:HE22	10	0.12	0.01	0.13
(1,400)	1:A:392:HIS:HB3	1:A:394:GLN:HE22	10	0.12	0.01	0.13
(1,574)	1:A:406:GLY:HA2	1:A:407:VAL:HA	8	0.21	0.03	0.2

[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)
(1,570)	1:A:406:GLY:H	1:A:407:VAL:H	14	0.56
(1,570)	1:A:406:GLY:H	1:A:407:VAL:H	17	0.56
(1,570)	1:A:406:GLY:H	1:A:407:VAL:H	19	0.55
(1,570)	1:A:406:GLY:H	1:A:407:VAL:H	13	0.53
(1,570)	1:A:406:GLY:H	1:A:407:VAL:H	22	0.52
(1,570)	1:A:406:GLY:H	1:A:407:VAL:H	8	0.51
(1,570)	1:A:406:GLY:H	1:A:407:VAL:H	15	0.5
(1,85)	1:A:375:LYS:HA	1:A:403:ASP:H	20	0.33
(1,530)	1:A:401:ASP:H	1:A:403:ASP:H	11	0.3
(1,530)	1:A:401:ASP:H	1:A:403:ASP:H	21	0.29

10 Dihedral-angle violation analysis

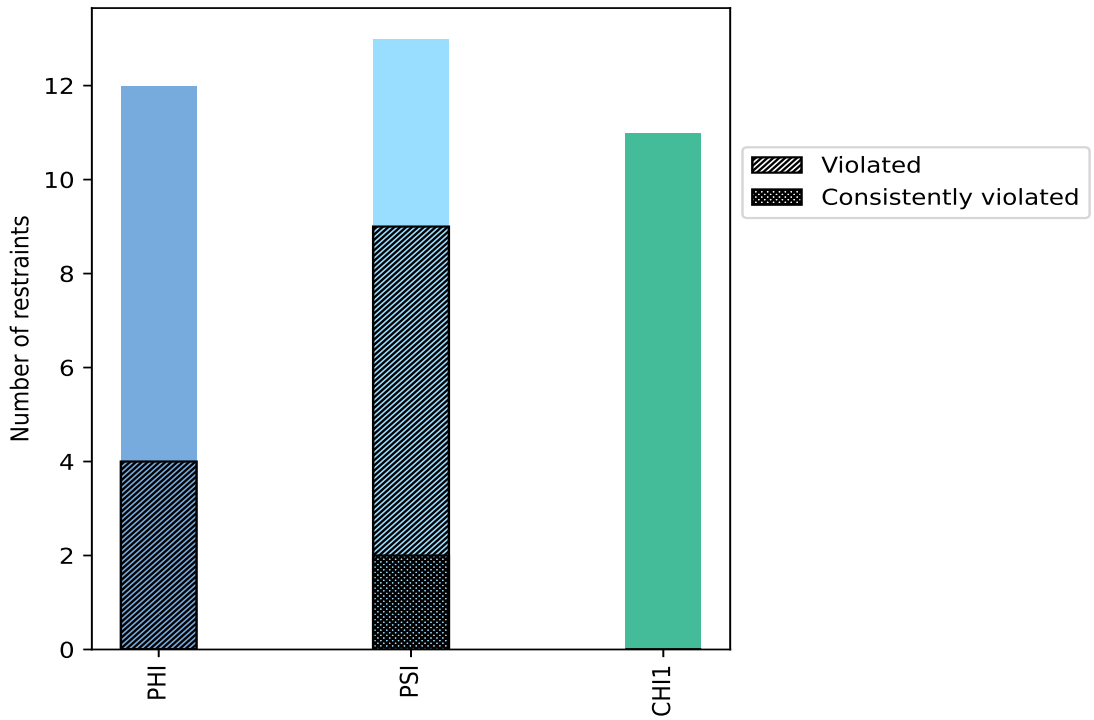
10.1 Summary of dihedral-angle violations

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]
PHI	12	33.3	4	33.3	11.1	0	0.0	0.0
PSI	13	36.1	9	69.2	25.0	2	15.4	5.6
CHI1	11	30.6	0	0.0	0.0	0	0.0	0.0
Total	36	100.0	13	36.1	36.1	2	5.6	5.6

[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



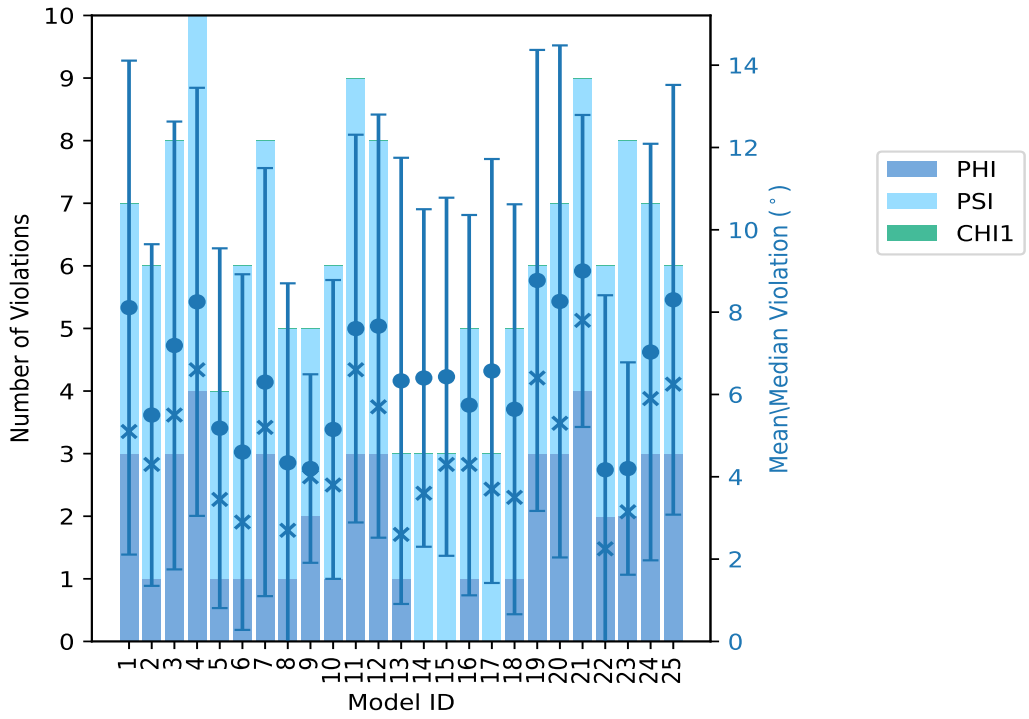
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PHI	PSI	CHI1	Total				
1	3	4	0	7	8.11	19.9	6.0	5.1
2	1	5	0	6	5.5	14.2	4.15	4.3
3	3	5	0	8	7.19	17.4	5.44	5.5
4	4	6	0	10	8.25	18.4	5.2	6.6
5	1	3	0	4	5.18	12.3	4.37	3.45
6	1	5	0	6	4.6	14.2	4.32	2.9
7	3	5	0	8	6.3	18.3	5.2	5.2
8	1	4	0	5	4.34	12.9	4.36	2.7
9	2	3	0	5	4.2	7.7	2.29	4.0
10	1	5	0	6	5.15	11.9	3.63	3.8
11	3	6	0	9	7.6	16.0	4.71	6.6
12	3	5	0	8	7.66	17.8	5.14	5.7
13	1	2	0	3	6.33	14.0	5.42	2.6
14	0	3	0	3	6.4	12.2	4.1	3.6
15	0	3	0	3	6.43	12.5	4.35	4.3
16	1	4	0	5	5.74	14.8	4.62	4.3
17	0	3	0	3	6.57	13.8	5.15	3.7
18	1	4	0	5	5.64	15.5	4.98	3.5
19	3	3	0	6	8.77	19.3	5.6	6.4
20	3	4	0	7	8.26	21.7	6.22	5.3
21	4	5	0	9	9.0	16.6	3.79	7.8
22	2	4	0	6	4.17	13.4	4.24	2.25
23	2	6	0	8	4.2	9.8	2.58	3.15
24	3	4	0	7	7.03	18.3	5.06	5.9
25	3	3	0	6	8.3	19.7	5.22	6.25

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	
PHI	PSI	CHI1	Total	Count[1]	%
0	2	0	2	1	4.0
1	0	0	1	2	8.0
0	0	0	0	3	12.0
0	0	0	0	4	16.0
0	0	0	0	5	20.0
0	2	0	2	6	24.0
0	0	0	0	7	28.0
0	0	0	0	8	32.0
0	1	0	1	9	36.0
0	0	0	0	10	40.0
1	0	0	1	11	44.0

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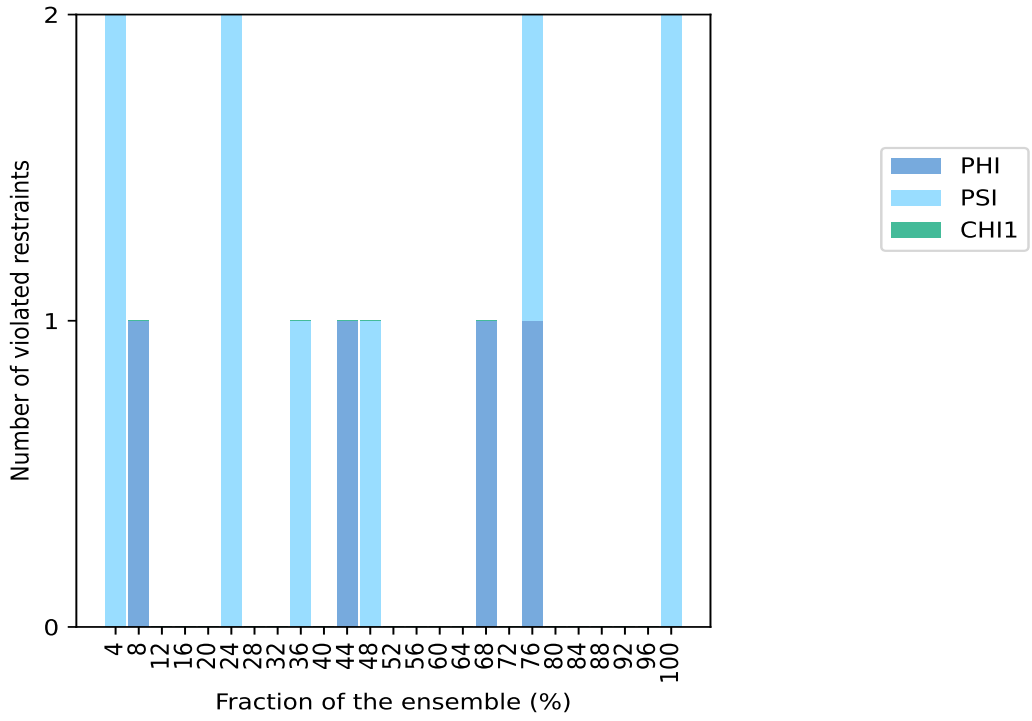
Number of violated restraints				Fraction of the ensemble	
PHI	PSI	CHI1	Total	Count[1]	%
0	1	0	1	12	48.0
0	0	0	0	13	52.0
0	0	0	0	14	56.0
0	0	0	0	15	60.0
0	0	0	0	16	64.0
1	0	0	1	17	68.0
0	0	0	0	18	72.0
1	1	0	2	19	76.0
0	0	0	0	20	80.0
0	0	0	0	21	84.0
0	0	0	0	22	88.0
0	0	0	0	23	92.0
0	0	0	0	24	96.0
0	2	0	2	25	100.0

[1] Number of models with violations

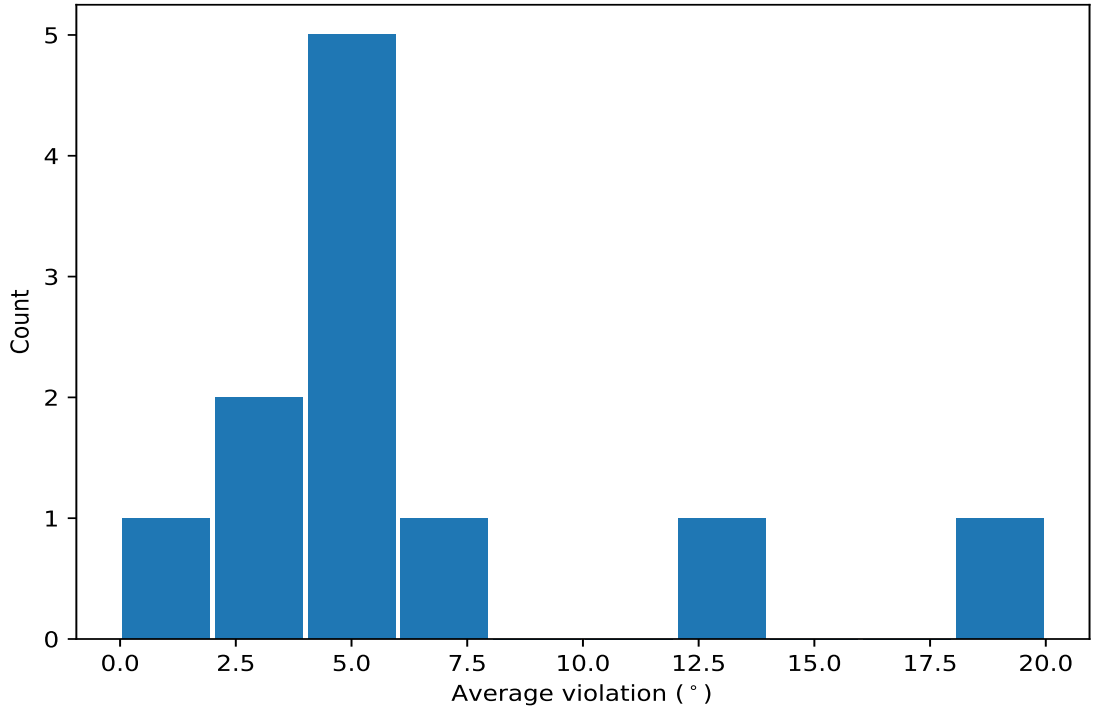
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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



10.4.2 Table: Most violated dihedral-angle restraints

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

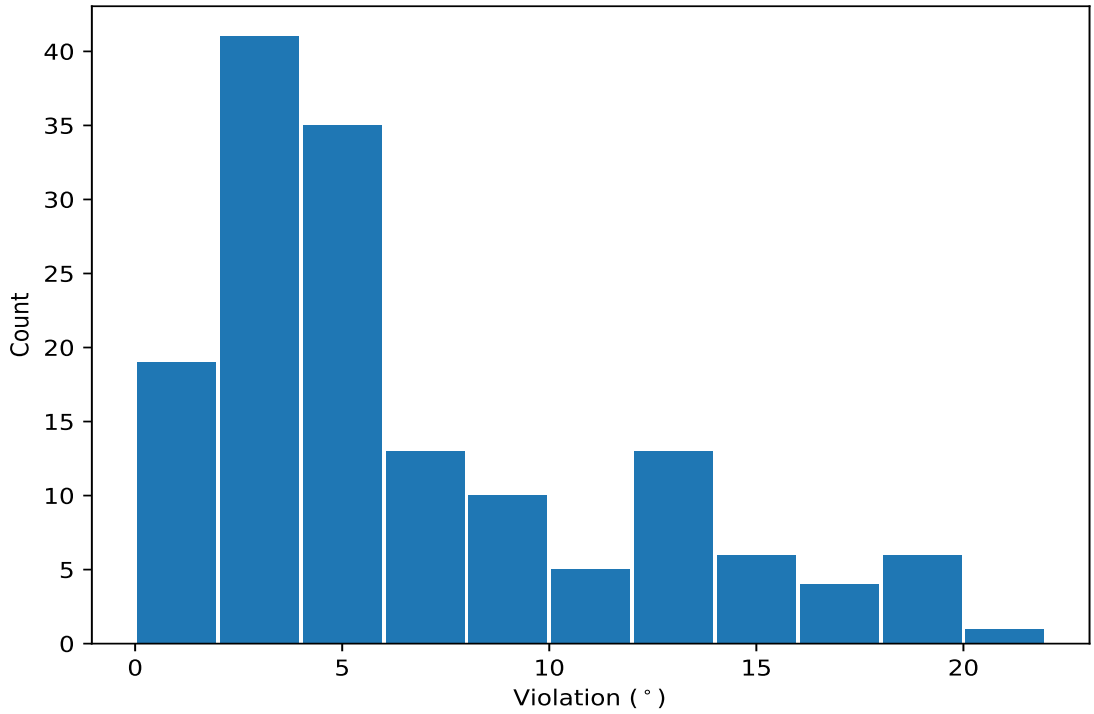
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,14)	1:A:398:HIS:N	1:A:398:HIS:CA	1:A:398:HIS:C	1:A:399:PRO:N	25	12.37	2.28	12.9
(1,17)	1:A:400:GLY:N	1:A:400:GLY:CA	1:A:400:GLY:C	1:A:401:ASP:N	25	4.52	1.36	4.2
(1,2)	1:A:391:VAL:N	1:A:391:VAL:CA	1:A:391:VAL:C	1:A:392:HIS:N	19	5.84	2.91	6.6
(1,13)	1:A:397:SER:C	1:A:398:HIS:N	1:A:398:HIS:CA	1:A:398:HIS:C	19	3.69	1.33	4.0
(1,18)	1:A:400:GLY:C	1:A:401:ASP:N	1:A:401:ASP:CA	1:A:401:ASP:C	17	4.06	2.66	3.5
(1,15)	1:A:399:PRO:N	1:A:399:PRO:CA	1:A:399:PRO:C	1:A:400:GLY:N	12	1.96	0.64	2.0
(1,1)	1:A:390:PRO:C	1:A:391:VAL:N	1:A:391:VAL:CA	1:A:391:VAL:C	11	18.49	1.54	18.3
(1,10)	1:A:396:PHE:N	1:A:396:PHE:CA	1:A:396:PHE:C	1:A:397:SER:N	9	3.34	1.1	3.3
(1,23)	1:A:403:ASP:N	1:A:403:ASP:CA	1:A:403:ASP:C	1:A:404:TYR:N	6	6.25	4.29	5.6
(1,25)	1:A:404:TYR:N	1:A:404:TYR:CA	1:A:404:TYR:C	1:A:405:GLY:N	6	5.6	2.26	6.2

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1)	1:A:390:PRO:C	1:A:391:VAL:N	1:A:391:VAL:CA	1:A:391:VAL:C	20	21.7
(1,1)	1:A:390:PRO:C	1:A:391:VAL:N	1:A:391:VAL:CA	1:A:391:VAL:C	1	19.9
(1,1)	1:A:390:PRO:C	1:A:391:VAL:N	1:A:391:VAL:CA	1:A:391:VAL:C	25	19.7
(1,1)	1:A:390:PRO:C	1:A:391:VAL:N	1:A:391:VAL:CA	1:A:391:VAL:C	19	19.3
(1,1)	1:A:390:PRO:C	1:A:391:VAL:N	1:A:391:VAL:CA	1:A:391:VAL:C	4	18.4
(1,1)	1:A:390:PRO:C	1:A:391:VAL:N	1:A:391:VAL:CA	1:A:391:VAL:C	7	18.3
(1,1)	1:A:390:PRO:C	1:A:391:VAL:N	1:A:391:VAL:CA	1:A:391:VAL:C	24	18.3
(1,1)	1:A:390:PRO:C	1:A:391:VAL:N	1:A:391:VAL:CA	1:A:391:VAL:C	12	17.8
(1,1)	1:A:390:PRO:C	1:A:391:VAL:N	1:A:391:VAL:CA	1:A:391:VAL:C	3	17.4
(1,1)	1:A:390:PRO:C	1:A:391:VAL:N	1:A:391:VAL:CA	1:A:391:VAL:C	21	16.6