



wwPDB NMR Structure Validation Summary Report ⓘ

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BMRB ID : 19977
Title : Solution structure human HCN2 CNBD in the cAMP-unbound state
Authors : Saponaro, A.; Pauleta, S.R.; Cantini, F.; Matzapetakis, M.; Hammann, C.;
Banci, L.; Thiel, G.; Santoro, B.; Moroni, A.
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This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

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

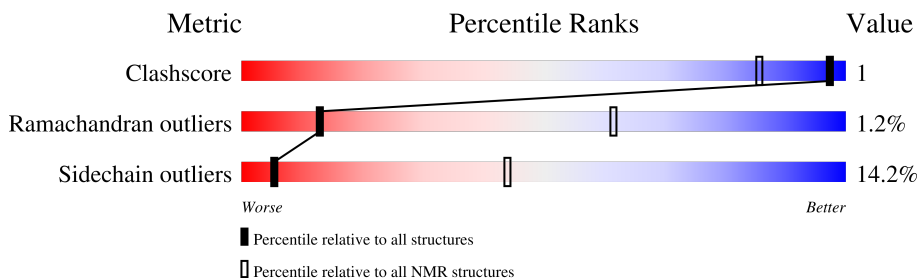
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 87%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	158	 65% 12% 11% 12%

2 Ensemble composition and analysis i

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:535-A:655 (121)	1.33	5

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 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2252 atoms, of which 1139 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	139	2252	709	1139	195	200	9	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	515	GLY	-	expression tag	UNP Q9UL51
A	516	PRO	-	expression tag	UNP Q9UL51
A	517	SER	-	expression tag	UNP Q9UL51
A	518	SER	-	expression tag	UNP Q9UL51
A	519	PRO	-	expression tag	UNP Q9UL51
A	520	MET	-	expression tag	UNP Q9UL51

5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, molecular dynamics*.

Of the 500 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
Amber	refinement	12
CANDID	structure solution	
CYANA	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	1886
Number of shifts mapped to atoms	1673
Number of unparsed shifts	0
Number of shifts with mapping errors	213
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

6 Model quality i

6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.86±0.02	0±0/987 (0.0± 0.0%)	1.50±0.04	4±2/1328 (0.3± 0.2%)
All	All	0.86	0/19740 (0.0%)	1.50	83/26560 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	3.5±1.6
All	All	0	69

There are no bond-length outliers.

5 of 30 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	583	PHE	CA-CB-CG	11.99	125.79	113.80	18	11
1	A	596	ASN	CA-CB-CG	9.95	122.55	112.60	19	17
1	A	638	PHE	CA-CB-CG	8.89	122.69	113.80	3	6
1	A	607	PHE	CA-CB-CG	6.03	119.83	113.80	17	3
1	A	622	VAL	N-CA-C	5.91	115.62	108.06	16	1

There are no chirality outliers.

5 of 19 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	595	GLY	Peptide	16
1	A	590	SER	Peptide	14
1	A	599	MET	Peptide	11

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	606	TYR	Sidechain	4
1	A	545	PHE	Sidechain	4

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	968	981	981	1±1
All	All	19360	19620	19620	23

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 1.

5 of 10 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:612:LEU:HD23	1:A:635:VAL:HG22	0.62	1.71	17	6
1:A:637:ASN:O	1:A:641:VAL:HG12	0.57	2.00	18	2
1:A:564:VAL:HG11	1:A:627:TYR:CE1	0.48	2.42	9	5
1:A:591:VAL:HG12	1:A:599:MET:C	0.48	2.33	17	2
1:A:613:LEU:HD13	1:A:613:LEU:H	0.45	1.72	8	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	121/158 (77%)	115±1 (95±1%)	4±1 (3±1%)	2±1 (1±1%)	13	61
All	All	2420/3160 (77%)	2307 (95%)	83 (3%)	30 (1%)	13	61

5 of 8 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	575	GLY	15
1	A	610	ILE	5
1	A	612	LEU	4
1	A	609	GLU	2
1	A	535	CYS	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	106/139 (76%)	91±3 (86±3%)	15±3 (14±3%)	5 44
All	All	2120/2780 (76%)	1820 (86%)	300 (14%)	5 44

5 of 58 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	539	VAL	20
1	A	561	LYS	20
1	A	594	LYS	20
1	A	597	LYS	18
1	A	593	THR	13

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](#)

There are no ligands in this entry.

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 i

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping i

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	1886
Number of shifts mapped to atoms	1673
Number of unparsed shifts	0
Number of shifts with mapping errors	213
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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 213) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	516	PRO	HA	4.511	0.020	1
1	A	516	PRO	HB2	2.303	0.020	2
1	A	516	PRO	HB3	2.103	0.020	2
1	A	516	PRO	HD2	3.484	0.020	2
1	A	516	PRO	HD3	3.44	0.020	2
1	A	516	PRO	HG2	1.879	0.020	2
1	A	516	PRO	HG3	1.771	0.020	2
1	A	516	PRO	CA	62.224	0.3	1
1	A	516	PRO	CB	34.52	0.3	1
1	A	516	PRO	CD	50.251	0.3	1
1	A	516	PRO	CG	24.622	0.3	1
1	A	517	SER	HA	4.416	0.020	1
1	A	517	SER	HB2	3.8	0.020	1
1	A	517	SER	HB3	3.8	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	517	SER	C	174.078	0.3	1
1	A	517	SER	CA	58.273	0.3	1
1	A	517	SER	CB	63.721	0.3	1
1	A	518	SER	H	8.221	0.020	1
1	A	518	SER	HA	3.796	0.020	1
1	A	518	SER	HB2	3.798	0.020	1
1	A	518	SER	HB3	3.798	0.020	1
1	A	518	SER	CA	56.265	0.3	1
1	A	518	SER	CB	63.262	0.3	1
1	A	518	SER	N	118.569	0.3	1
1	A	519	PRO	HA	4.335	0.020	1
1	A	519	PRO	HB2	2.24	0.020	2
1	A	519	PRO	HB3	1.858	0.020	2
1	A	519	PRO	HD2	3.747	0.020	2
1	A	519	PRO	HD3	3.656	0.020	2
1	A	519	PRO	HG2	1.947	0.020	1
1	A	519	PRO	HG3	1.947	0.020	1
1	A	519	PRO	C	177.009	0.3	1
1	A	519	PRO	CA	63.448	0.3	1
1	A	519	PRO	CB	31.854	0.3	1
1	A	519	PRO	CD	50.595	0.3	1
1	A	519	PRO	CG	27.245	0.3	1
1	A	520	MET	H	8.258	0.020	1
1	A	520	MET	HA	4.321	0.020	1
1	A	520	MET	HB2	1.985	0.020	2
1	A	520	MET	HB3	1.912	0.020	2
1	A	520	MET	HG2	2.513	0.020	2
1	A	520	MET	HG3	2.466	0.020	2
1	A	520	MET	C	176.293	0.3	1
1	A	520	MET	CA	55.805	0.3	1
1	A	520	MET	CB	32.709	0.3	1
1	A	520	MET	CG	31.878	0.3	1
1	A	520	MET	N	119.429	0.3	1
1	A	521	GLU	H	8.21	0.020	1
1	A	521	GLU	HA	4.198	0.020	1
1	A	521	GLU	HB2	1.944	0.020	2
1	A	521	GLU	HB3	1.858	0.020	2
1	A	521	GLU	HG2	2.152	0.020	1
1	A	521	GLU	HG3	2.152	0.020	1
1	A	521	GLU	C	176.319	0.3	1
1	A	521	GLU	CA	56.479	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	521	GLU	CB	30.1	0.3	1
1	A	521	GLU	CG	36.13	0.3	1
1	A	521	GLU	N	121.524	0.3	1
1	A	522	LEU	H	8.112	0.020	1
1	A	522	LEU	HA	4.253	0.020	1
1	A	522	LEU	HB2	1.502	0.020	1
1	A	522	LEU	HB3	1.502	0.020	1
1	A	522	LEU	HD11	0.832	0.020	1
1	A	522	LEU	HD12	0.832	0.020	1
1	A	522	LEU	HD13	0.832	0.020	1
1	A	522	LEU	HD21	0.772	0.020	1
1	A	522	LEU	HD22	0.772	0.020	1
1	A	522	LEU	HD23	0.772	0.020	1
1	A	522	LEU	HG	1.528	0.020	1
1	A	522	LEU	C	176.887	0.3	1
1	A	522	LEU	CA	55.161	0.3	1
1	A	522	LEU	CB	42.16	0.3	1
1	A	522	LEU	CD1	24.692	0.3	1
1	A	522	LEU	CD2	23.423	0.3	1
1	A	522	LEU	CG	26.779	0.3	1
1	A	522	LEU	N	122.766	0.3	1
1	A	523	ASN	H	8.286	0.020	1
1	A	523	ASN	HA	4.691	0.020	1
1	A	523	ASN	HB2	2.768	0.020	2
1	A	523	ASN	HB3	2.664	0.020	2
1	A	523	ASN	HD21	7.514	0.020	1
1	A	523	ASN	HD22	6.845	0.020	1
1	A	523	ASN	C	175.081	0.3	1
1	A	523	ASN	CA	53.023	0.3	1
1	A	523	ASN	CB	39.104	0.3	1
1	A	523	ASN	CG	176.659	0.3	1
1	A	523	ASN	N	118.606	0.3	1
1	A	523	ASN	ND2	112.953	0.3	1
1	A	524	GLY	H	8.061	0.020	1
1	A	524	GLY	HA2	3.987	0.020	1
1	A	524	GLY	HA3	3.987	0.020	1
1	A	524	GLY	CA	44.931	0.3	1
1	A	524	GLY	N	108.964	0.3	1
1	A	525	PRO	HA	4.443	0.020	1
1	A	525	PRO	HB2	2.243	0.020	2
1	A	525	PRO	HB3	2.183	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	525	PRO	HD2	3.514	0.020	1
1	A	525	PRO	HD3	3.514	0.020	1
1	A	525	PRO	HG2	1.948	0.020	2
1	A	525	PRO	HG3	1.899	0.020	2
1	A	525	PRO	C	177.141	0.3	1
1	A	525	PRO	CA	63.096	0.3	1
1	A	525	PRO	CB	32.16	0.3	1
1	A	525	PRO	CD	49.638	0.3	1
1	A	525	PRO	CG	26.909	0.3	1
1	A	526	LEU	H	8.203	0.020	1
1	A	526	LEU	HA	4.247	0.020	1
1	A	526	LEU	HB2	1.557	0.020	2
1	A	526	LEU	HB3	1.498	0.020	2
1	A	526	LEU	HD11	0.832	0.020	1
1	A	526	LEU	HD12	0.832	0.020	1
1	A	526	LEU	HD13	0.832	0.020	1
1	A	526	LEU	HD21	0.775	0.020	1
1	A	526	LEU	HD22	0.775	0.020	1
1	A	526	LEU	HD23	0.775	0.020	1
1	A	526	LEU	HG	1.531	0.020	1
1	A	526	LEU	C	177.423	0.3	1
1	A	526	LEU	CA	55.254	0.3	1
1	A	526	LEU	CB	42.118	0.3	1
1	A	526	LEU	CD1	24.733	0.3	1
1	A	526	LEU	CD2	23.518	0.3	1
1	A	526	LEU	CG	26.818	0.3	1
1	A	526	LEU	N	121.258	0.3	1
1	A	527	ARG	H	8.116	0.020	1
1	A	527	ARG	HA	4.165	0.020	1
1	A	527	ARG	HB2	1.753	0.020	2
1	A	527	ARG	HB3	1.713	0.020	2
1	A	527	ARG	HD2	3.116	0.020	1
1	A	527	ARG	HD3	3.116	0.020	1
1	A	527	ARG	HG2	1.556	0.020	1
1	A	527	ARG	HG3	1.556	0.020	1
1	A	527	ARG	C	176.456	0.3	1
1	A	527	ARG	CA	56.555	0.3	1
1	A	527	ARG	CB	30.478	0.3	1
1	A	527	ARG	CD	43.109	0.3	1
1	A	527	ARG	CG	26.943	0.3	1
1	A	527	ARG	N	121.455	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	528	GLU	H	8.338	0.020	1
1	A	528	GLU	HA	4.092	0.020	1
1	A	528	GLU	HB2	1.943	0.020	2
1	A	528	GLU	HB3	1.859	0.020	2
1	A	528	GLU	HG2	2.154	0.020	1
1	A	528	GLU	HG3	2.154	0.020	1
1	A	528	GLU	C	176.574	0.3	1
1	A	528	GLU	CA	57.209	0.3	1
1	A	528	GLU	CB	29.972	0.3	1
1	A	528	GLU	CG	36.194	0.3	1
1	A	528	GLU	N	121.28	0.3	1
1	A	529	GLU	H	8.366	0.020	1
1	A	529	GLU	HA	4.097	0.020	1
1	A	529	GLU	HB2	1.941	0.020	2
1	A	529	GLU	HB3	1.866	0.020	2
1	A	529	GLU	HG2	2.154	0.020	1
1	A	529	GLU	HG3	2.154	0.020	1
1	A	529	GLU	C	176.85	0.3	1
1	A	529	GLU	CA	57.056	0.3	1
1	A	529	GLU	CB	29.838	0.3	1
1	A	529	GLU	CG	36.171	0.3	1
1	A	529	GLU	N	120.988	0.3	1
1	A	530	ILE	H	7.941	0.020	1
1	A	530	ILE	HA	4.004	0.020	1
1	A	530	ILE	HB	1.803	0.020	1
1	A	530	ILE	HD11	0.719	0.020	1
1	A	530	ILE	HD12	0.719	0.020	1
1	A	530	ILE	HD13	0.719	0.020	1
1	A	530	ILE	HG12	1.375	0.020	2
1	A	530	ILE	HG13	1.093	0.020	2
1	A	530	ILE	HG21	0.789	0.020	1
1	A	530	ILE	HG22	0.789	0.020	1
1	A	530	ILE	HG23	0.789	0.020	1
1	A	530	ILE	C	176.611	0.3	1
1	A	530	ILE	CA	61.653	0.3	1
1	A	530	ILE	CB	38.119	0.3	1
1	A	530	ILE	CD1	12.603	0.3	1
1	A	530	ILE	CG1	27.436	0.3	1
1	A	530	ILE	CG2	17.405	0.3	1
1	A	530	ILE	N	121.269	0.3	1
1	A	531	VAL	H	7.952	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	531	VAL	HA	3.862	0.020	1
1	A	531	VAL	HB	1.92	0.020	1
1	A	531	VAL	HG11	0.767	0.020	1
1	A	531	VAL	HG12	0.767	0.020	1
1	A	531	VAL	HG13	0.767	0.020	1
1	A	531	VAL	HG21	0.767	0.020	1
1	A	531	VAL	HG22	0.767	0.020	1
1	A	531	VAL	HG23	0.767	0.020	1
1	A	531	VAL	C	176.308	0.3	1
1	A	531	VAL	CA	63.257	0.3	1
1	A	531	VAL	CB	32.11	0.3	1
1	A	531	VAL	CG1	20.932	0.3	1
1	A	531	VAL	N	122.87	0.3	1
1	A	532	ASN	H	8.267	0.020	1
1	A	532	ASN	HA	4.502	0.020	1
1	A	532	ASN	HB2	2.682	0.020	1
1	A	532	ASN	HB3	2.682	0.020	1
1	A	532	ASN	HD21	7.516	0.020	1
1	A	532	ASN	HD22	6.786	0.020	1
1	A	532	ASN	C	175.26	0.3	1
1	A	532	ASN	CA	53.718	0.3	1
1	A	532	ASN	CB	38.469	0.3	1
1	A	532	ASN	N	120.311	0.3	1
1	A	532	ASN	ND2	112.632	0.3	1
1	A	533	PHE	H	8.055	0.020	1
1	A	533	PHE	HA	4.289	0.020	1
1	A	533	PHE	HB2	3.105	0.020	2
1	A	533	PHE	HB3	2.973	0.020	2
1	A	533	PHE	HD1	7.247	0.020	1
1	A	533	PHE	HD2	7.247	0.020	1
1	A	533	PHE	HE1	7.181	0.020	1
1	A	533	PHE	HE2	7.181	0.020	1
1	A	533	PHE	CA	59.097	0.3	1
1	A	533	PHE	CB	39.05	0.3	1
1	A	533	PHE	N	120.952	0.3	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	152	0.07 ± 0.20	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	142	0.12 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	131	0.15 ± 0.19	None needed (< 0.5 ppm)
^{15}N	139	0.49 ± 0.43	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 87%, i.e. 1479 atoms were assigned a chemical shift out of a possible 1698. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	576/605 (95%)	240/246 (98%)	224/242 (93%)	112/117 (96%)
Sidechain	839/952 (88%)	570/620 (92%)	261/290 (90%)	8/42 (19%)
Aromatic	64/141 (45%)	63/68 (93%)	1/72 (1%)	0/1 (0%)
Overall	1479/1698 (87%)	873/934 (93%)	486/604 (80%)	120/160 (75%)

7.1.4 Statistically unusual chemical shifts [i](#)

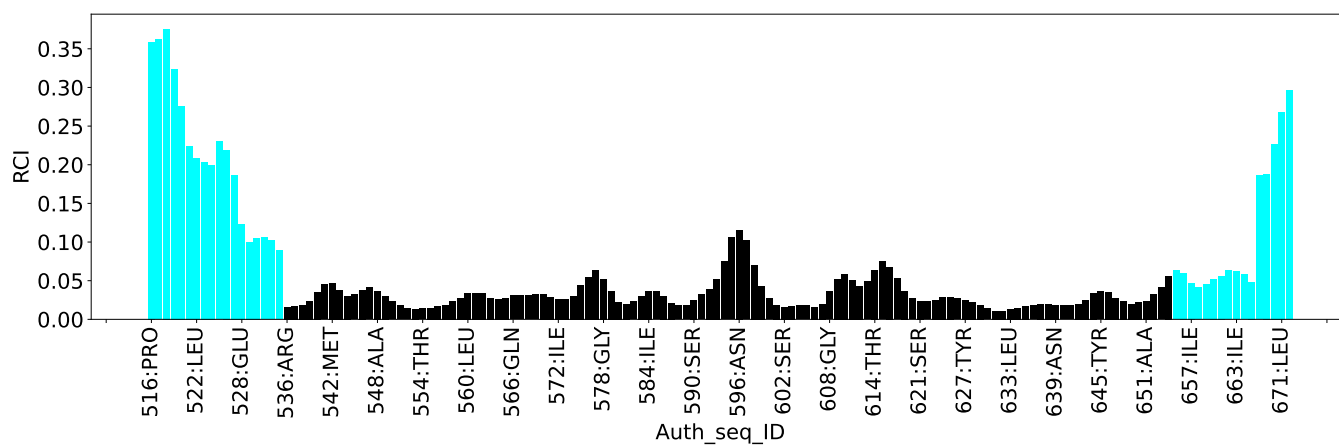
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	582	TYR	HB3	0.61	0.93 – 4.76	-5.8
1	A	571	ILE	HG13	-1.10	-0.82 – 3.23	-5.7

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	1687
Intra-residue ($ i-j =0$)	406
Sequential ($ i-j =1$)	534
Medium range ($ i-j >1$ and $ i-j <5$)	262
Long range ($ i-j \geq 5$)	449
Inter-chain	0
Hydrogen bond restraints	36
Disulfide bond restraints	0
Total dihedral-angle restraints	198
Number of unmapped restraints	103
Number of restraints per residue	11.9
Number of long range restraints per residue ¹	3.1

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)	5.5	0.2
0.2-0.5 (Medium)	6.8	0.5
>0.5 (Large)	9.7	2.12

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)	14.2	8.89
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis [i](#)

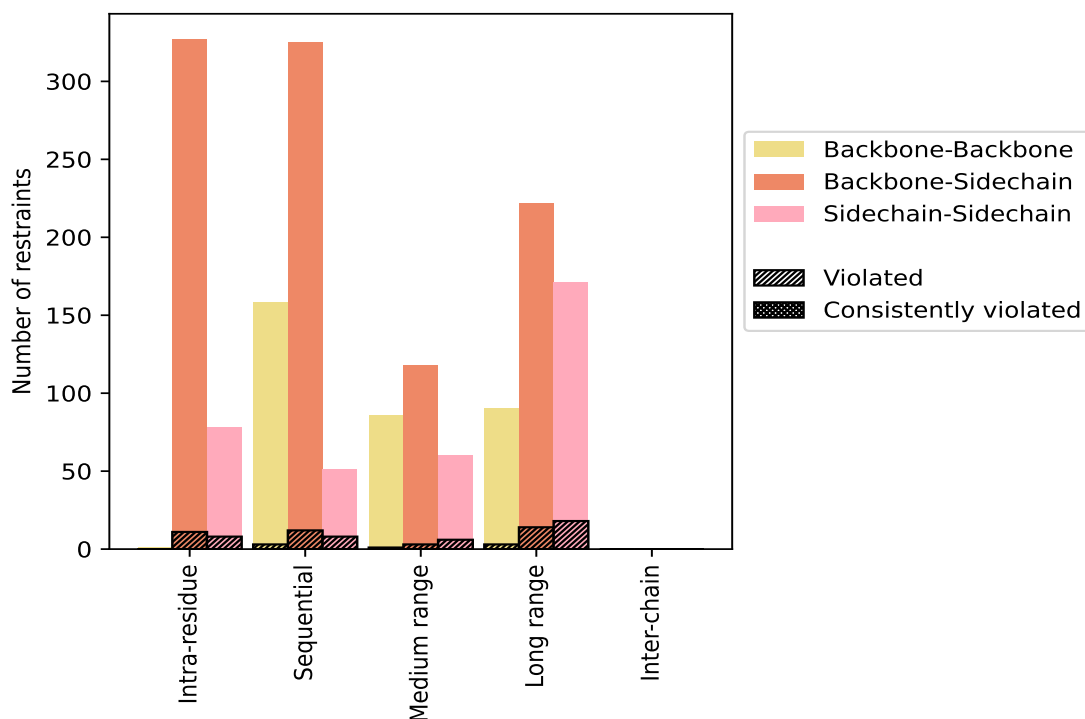
9.1 Summary of distance violations [i](#)

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	406	24.1	19	4.7	1.1	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	327	19.4	11	3.4	0.7	0	0.0	0.0
Sidechain-Sidechain	78	4.6	8	10.3	0.5	0	0.0	0.0
Sequential ($i-j =1$)	534	31.7	23	4.3	1.4	0	0.0	0.0
Backbone-Backbone	158	9.4	3	1.9	0.2	0	0.0	0.0
Backbone-Sidechain	325	19.3	12	3.7	0.7	0	0.0	0.0
Sidechain-Sidechain	51	3.0	8	15.7	0.5	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	262	15.5	10	3.8	0.6	0	0.0	0.0
Backbone-Backbone	86	5.1	1	1.2	0.1	0	0.0	0.0
Backbone-Sidechain	116	6.9	3	2.6	0.2	0	0.0	0.0
Sidechain-Sidechain	60	3.6	6	10.0	0.4	0	0.0	0.0
Long range ($i-j \geq 5$)	449	26.6	35	7.8	2.1	0	0.0	0.0
Backbone-Backbone	90	5.3	3	3.3	0.2	0	0.0	0.0
Backbone-Sidechain	188	11.1	14	7.4	0.8	0	0.0	0.0
Sidechain-Sidechain	171	10.1	18	10.5	1.1	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	36	2.1	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	1687	100.0	87	5.2	5.2	0	0.0	0.0
Backbone-Backbone	335	19.9	7	2.1	0.4	0	0.0	0.0
Backbone-Sidechain	992	58.8	40	4.0	2.4	0	0.0	0.0
Sidechain-Sidechain	360	21.3	40	11.1	2.4	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 disulfid 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	6	7	9	0	27	0.45	1.65	0.44	0.2
2	1	3	6	10	0	20	0.6	1.35	0.4	0.56
3	3	6	4	9	0	22	0.58	2.09	0.56	0.36
4	3	7	6	10	0	26	0.64	1.82	0.52	0.55
5	2	7	6	10	0	25	0.67	1.73	0.5	0.45
6	3	3	7	13	0	26	0.55	2.08	0.5	0.42
7	7	3	6	10	0	26	0.51	2.12	0.49	0.38
8	3	6	3	10	0	22	0.55	1.5	0.36	0.49
9	2	4	5	19	0	30	0.44	1.53	0.35	0.33
10	0	5	5	7	0	17	0.57	1.29	0.38	0.55

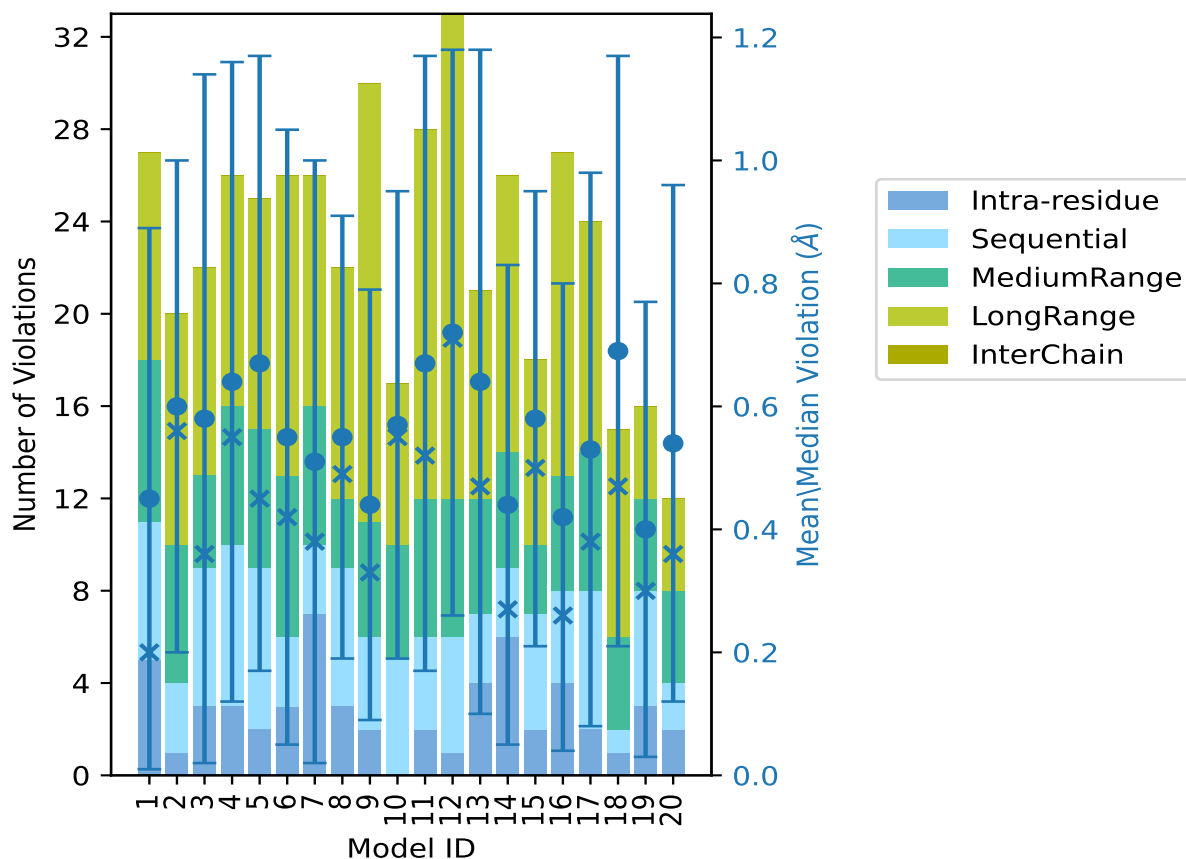
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵					
11	2	4	6	16	0	28	0.67	1.82	0.5	0.52
12	1	5	6	21	0	33	0.72	1.75	0.46	0.71
13	4	3	5	9	0	21	0.64	2.11	0.54	0.47
14	6	3	5	12	0	26	0.44	1.52	0.39	0.27
15	2	5	3	8	0	18	0.58	1.52	0.37	0.5
16	4	4	5	14	0	27	0.42	1.45	0.38	0.26
17	2	6	6	10	0	24	0.53	1.84	0.45	0.38
18	1	1	4	9	0	15	0.69	1.8	0.48	0.47
19	3	5	4	4	0	16	0.4	1.42	0.37	0.3
20	2	2	4	4	0	12	0.54	1.51	0.42	0.36

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 [i](#)



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

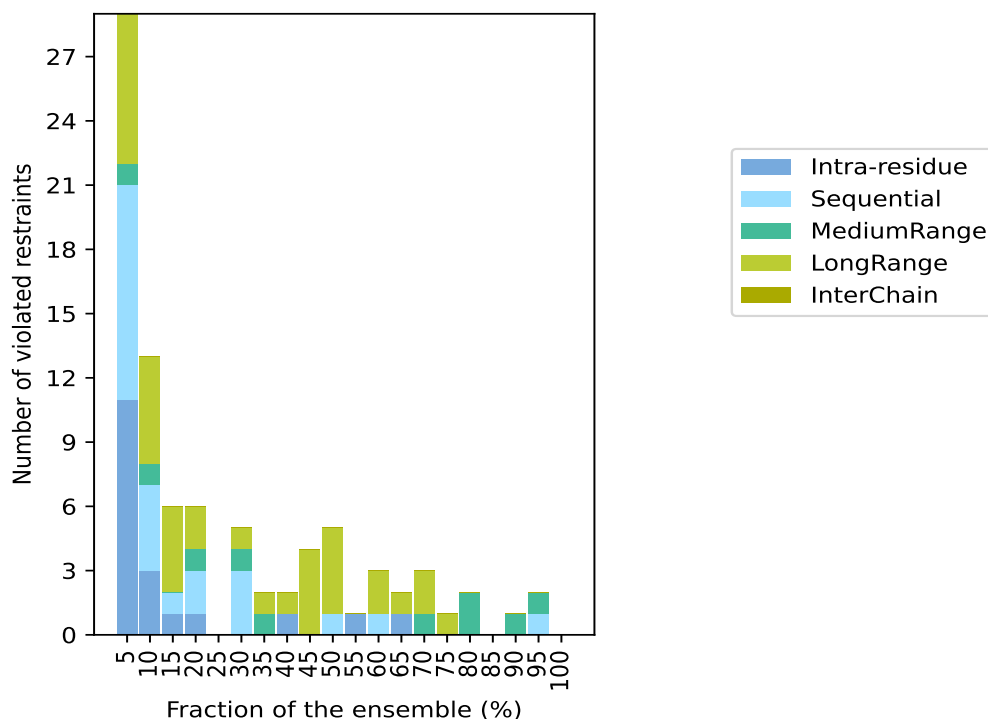
9.3 Distance violation statistics for the ensemble

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, 1564(IR:387, SQ:511, MR:252, LR:414, 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	%
11	10	1	7	0	29	1	5.0
3	4	1	5	0	13	2	10.0
1	1	0	4	0	6	3	15.0
1	2	1	2	0	6	4	20.0
0	0	0	0	0	0	5	25.0
0	3	1	1	0	5	6	30.0
0	0	1	1	0	2	7	35.0
1	0	0	1	0	2	8	40.0
0	0	0	4	0	4	9	45.0
0	1	0	4	0	5	10	50.0
1	0	0	0	0	1	11	55.0
0	1	0	2	0	3	12	60.0
1	0	0	1	0	2	13	65.0
0	0	1	2	0	3	14	70.0
0	0	0	1	0	1	15	75.0
0	0	2	0	0	2	16	80.0
0	0	0	0	0	0	17	85.0
0	0	1	0	0	1	18	90.0
0	1	1	0	0	2	19	95.0
0	0	0	0	0	0	20	100.0

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

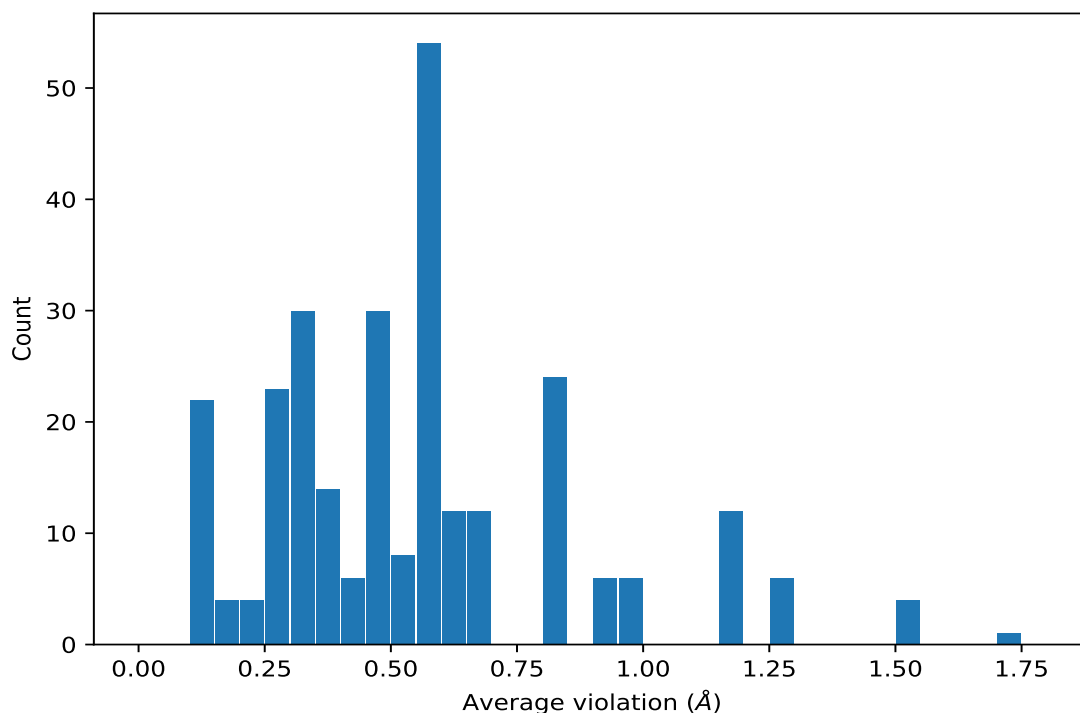
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,1484)	1:648:A:MET:HE1	1:652:A:PHE:HD1	19	0.98	0.45	0.95
(1,1484)	1:648:A:MET:HE1	1:652:A:PHE:HD2	19	0.98	0.45	0.95
(1,1484)	1:648:A:MET:HE2	1:652:A:PHE:HD1	19	0.98	0.45	0.95
(1,1484)	1:648:A:MET:HE2	1:652:A:PHE:HD2	19	0.98	0.45	0.95
(1,1484)	1:648:A:MET:HE3	1:652:A:PHE:HD1	19	0.98	0.45	0.95
(1,1484)	1:648:A:MET:HE3	1:652:A:PHE:HD2	19	0.98	0.45	0.95
(1,1039)	1:592:A:LEU:HD11	1:593:A:THR:H	19	0.67	0.22	0.72
(1,1039)	1:592:A:LEU:HD12	1:593:A:THR:H	19	0.67	0.22	0.72
(1,1039)	1:592:A:LEU:HD13	1:593:A:THR:H	19	0.67	0.22	0.72
(1,1039)	1:592:A:LEU:HD21	1:593:A:THR:H	19	0.67	0.22	0.72
(1,1039)	1:592:A:LEU:HD22	1:593:A:THR:H	19	0.67	0.22	0.72
(1,1039)	1:592:A:LEU:HD23	1:593:A:THR:H	19	0.67	0.22	0.72
(1,994)	1:590:A:SER:HB3	1:592:A:LEU:HD11	18	1.18	0.54	1.38
(1,994)	1:590:A:SER:HB3	1:592:A:LEU:HD12	18	1.18	0.54	1.38
(1,994)	1:590:A:SER:HB3	1:592:A:LEU:HD13	18	1.18	0.54	1.38
(1,994)	1:590:A:SER:HB3	1:592:A:LEU:HD21	18	1.18	0.54	1.38

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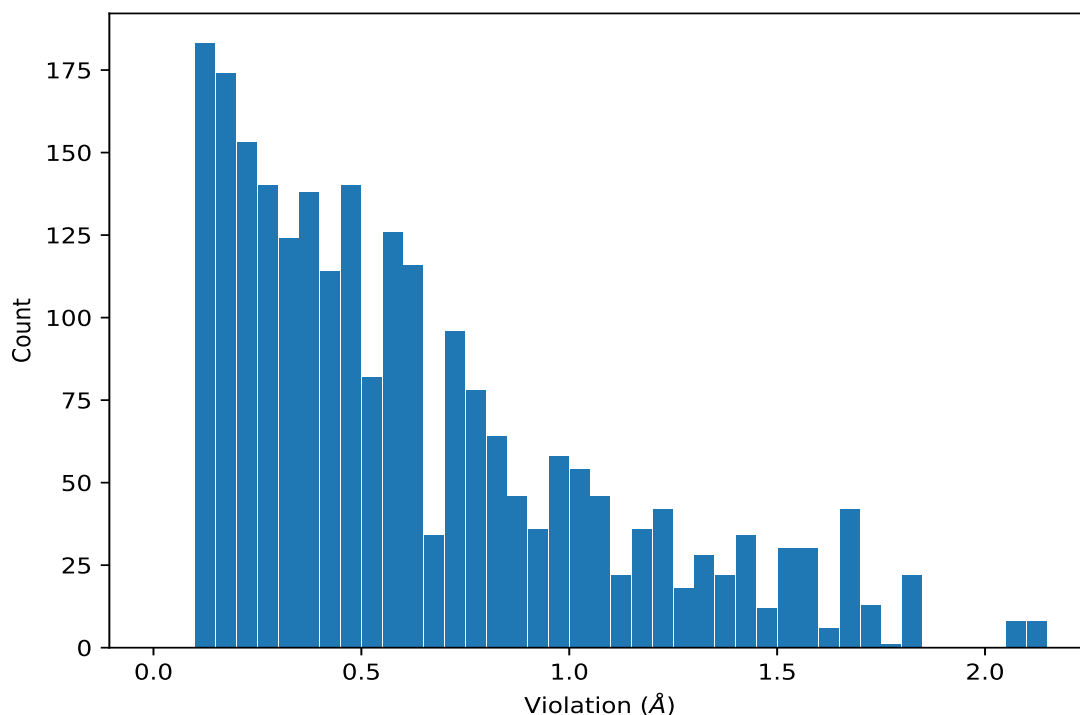
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,994)	1:590:A:SER:HB3	1:592:A:LEU:HD22	18	1.18	0.54	1.38
(1,994)	1:590:A:SER:HB3	1:592:A:LEU:HD23	18	1.18	0.54	1.38
(1,1514)	1:650:A:ARG:HD2	1:654:A:THR:HG21	16	1.17	0.52	1.28
(1,1514)	1:650:A:ARG:HD2	1:654:A:THR:HG22	16	1.17	0.52	1.28
(1,1514)	1:650:A:ARG:HD2	1:654:A:THR:HG23	16	1.17	0.52	1.28
(1,1514)	1:650:A:ARG:HD3	1:654:A:THR:HG21	16	1.17	0.52	1.28
(1,1514)	1:650:A:ARG:HD3	1:654:A:THR:HG22	16	1.17	0.52	1.28
(1,1514)	1:650:A:ARG:HD3	1:654:A:THR:HG23	16	1.17	0.52	1.28
(1,1581)	1:656:A:ALA:HB1	1:659:A:ARG:HD2	16	0.85	0.37	0.91
(1,1581)	1:656:A:ALA:HB1	1:659:A:ARG:HD3	16	0.85	0.37	0.91
(1,1581)	1:656:A:ALA:HB2	1:659:A:ARG:HD2	16	0.85	0.37	0.91
(1,1581)	1:656:A:ALA:HB2	1:659:A:ARG:HD3	16	0.85	0.37	0.91
(1,1581)	1:656:A:ALA:HB3	1:659:A:ARG:HD2	16	0.85	0.37	0.91
(1,1581)	1:656:A:ALA:HB3	1:659:A:ARG:HD3	16	0.85	0.37	0.91
(1,449)	1:560:A:LEU:HA	1:633:A:LEU:HD11	15	0.67	0.14	0.71
(1,449)	1:560:A:LEU:HA	1:633:A:LEU:HD12	15	0.67	0.14	0.71
(1,449)	1:560:A:LEU:HA	1:633:A:LEU:HD13	15	0.67	0.14	0.71
(1,449)	1:560:A:LEU:HA	1:633:A:LEU:HD21	15	0.67	0.14	0.71
(1,449)	1:560:A:LEU:HA	1:633:A:LEU:HD22	15	0.67	0.14	0.71
(1,449)	1:560:A:LEU:HA	1:633:A:LEU:HD23	15	0.67	0.14	0.71
(1,990)	1:590:A:SER:HB2	1:592:A:LEU:HD11	14	1.26	0.32	1.37
(1,990)	1:590:A:SER:HB2	1:592:A:LEU:HD12	14	1.26	0.32	1.37
(1,990)	1:590:A:SER:HB2	1:592:A:LEU:HD13	14	1.26	0.32	1.37
(1,990)	1:590:A:SER:HB2	1:592:A:LEU:HD21	14	1.26	0.32	1.37
(1,990)	1:590:A:SER:HB2	1:592:A:LEU:HD22	14	1.26	0.32	1.37
(1,990)	1:590:A:SER:HB2	1:592:A:LEU:HD23	14	1.26	0.32	1.37
(1,1022)	1:591:A:VAL:HG21	1:600:A:LYS:HA	14	0.16	0.01	0.16
(1,1022)	1:591:A:VAL:HG22	1:600:A:LYS:HA	14	0.16	0.01	0.16
(1,1022)	1:591:A:VAL:HG23	1:600:A:LYS:HA	14	0.16	0.01	0.16
(1,986)	1:590:A:SER:HA	1:600:A:LYS:H	14	0.14	0.02	0.14
(1,145)	1:538:A:LEU:HD11	1:605:A:SER:H	13	0.62	0.37	0.53

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)
(1,701)	1:574:A:GLU:HG2	1:579:A:LYS:HD2	7	2.12
(1,701)	1:574:A:GLU:HG2	1:579:A:LYS:HD3	7	2.12
(1,701)	1:574:A:GLU:HG3	1:579:A:LYS:HD2	7	2.12
(1,701)	1:574:A:GLU:HG3	1:579:A:LYS:HD3	7	2.12
(1,701)	1:574:A:GLU:HG2	1:579:A:LYS:HD2	13	2.11
(1,701)	1:574:A:GLU:HG2	1:579:A:LYS:HD3	13	2.11
(1,701)	1:574:A:GLU:HG3	1:579:A:LYS:HD2	13	2.11
(1,701)	1:574:A:GLU:HG3	1:579:A:LYS:HD3	13	2.11
(1,701)	1:574:A:GLU:HG2	1:579:A:LYS:HD2	3	2.09
(1,701)	1:574:A:GLU:HG2	1:579:A:LYS:HD3	3	2.09
(1,701)	1:574:A:GLU:HG3	1:579:A:LYS:HD2	3	2.09
(1,701)	1:574:A:GLU:HG3	1:579:A:LYS:HD3	3	2.09
(1,701)	1:574:A:GLU:HG2	1:579:A:LYS:HD2	6	2.08
(1,701)	1:574:A:GLU:HG2	1:579:A:LYS:HD3	6	2.08
(1,701)	1:574:A:GLU:HG3	1:579:A:LYS:HD2	6	2.08
(1,701)	1:574:A:GLU:HG3	1:579:A:LYS:HD3	6	2.08
(1,701)	1:574:A:GLU:HG2	1:579:A:LYS:HD2	17	1.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,701)	1:574:A:GLU:HG2	1:579:A:LYS:HD3	17	1.84
(1,701)	1:574:A:GLU:HG3	1:579:A:LYS:HD2	17	1.84
(1,701)	1:574:A:GLU:HG3	1:579:A:LYS:HD3	17	1.84
(1,1484)	1:648:A:MET:HE1	1:652:A:PHE:HD1	4	1.82
(1,1484)	1:648:A:MET:HE1	1:652:A:PHE:HD2	4	1.82
(1,1484)	1:648:A:MET:HE2	1:652:A:PHE:HD1	4	1.82
(1,1484)	1:648:A:MET:HE2	1:652:A:PHE:HD2	4	1.82
(1,1484)	1:648:A:MET:HE3	1:652:A:PHE:HD1	4	1.82
(1,1484)	1:648:A:MET:HE3	1:652:A:PHE:HD2	4	1.82
(1,990)	1:590:A:SER:HB2	1:592:A:LEU:HD11	11	1.82
(1,990)	1:590:A:SER:HB2	1:592:A:LEU:HD12	11	1.82
(1,990)	1:590:A:SER:HB2	1:592:A:LEU:HD13	11	1.82
(1,990)	1:590:A:SER:HB2	1:592:A:LEU:HD21	11	1.82
(1,990)	1:590:A:SER:HB2	1:592:A:LEU:HD22	11	1.82
(1,990)	1:590:A:SER:HB2	1:592:A:LEU:HD23	11	1.82
(1,1514)	1:650:A:ARG:HD2	1:654:A:THR:HG21	18	1.8
(1,1514)	1:650:A:ARG:HD2	1:654:A:THR:HG22	18	1.8
(1,1514)	1:650:A:ARG:HD2	1:654:A:THR:HG23	18	1.8
(1,1514)	1:650:A:ARG:HD3	1:654:A:THR:HG21	18	1.8
(1,1514)	1:650:A:ARG:HD3	1:654:A:THR:HG22	18	1.8
(1,1514)	1:650:A:ARG:HD3	1:654:A:THR:HG23	18	1.8
(1,1336)	1:636:A:ASP:HB2	1:637:A:ASN:HD22	12	1.75
(1,1514)	1:650:A:ARG:HD2	1:654:A:THR:HG21	12	1.73

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

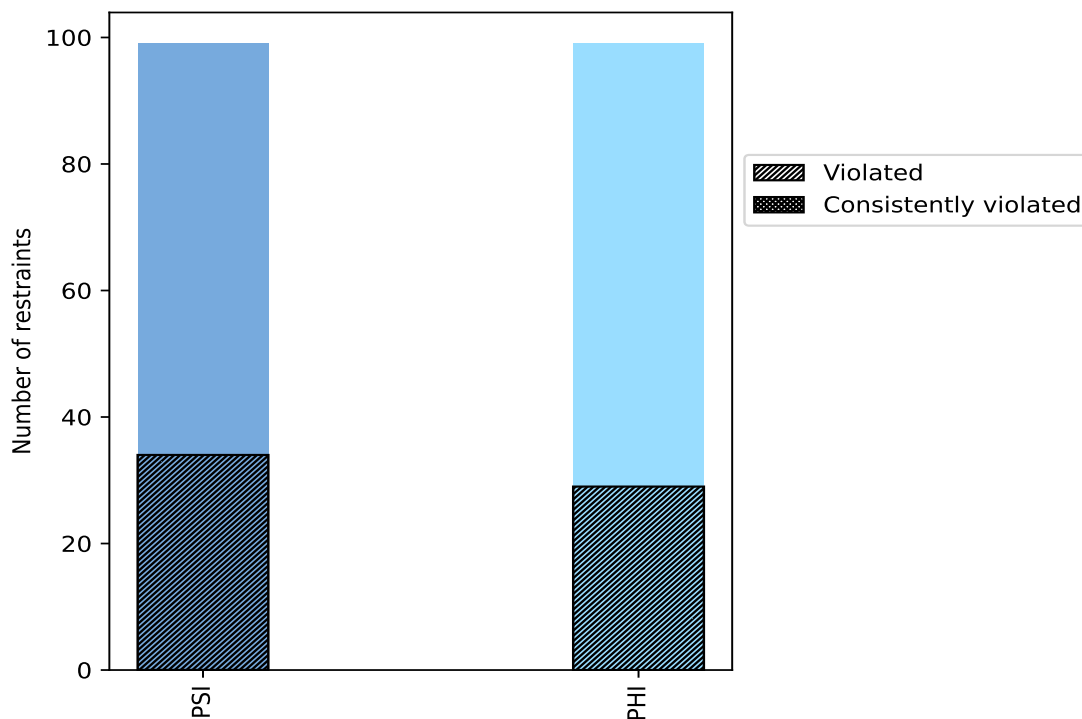
10.1 Summary of dihedral-angle violations [i](#)

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	99	50.0	34	34.3	17.2	0	0.0	0.0
PHI	99	50.0	29	29.3	14.6	0	0.0	0.0
Total	198	100.0	63	31.8	31.8	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](#)



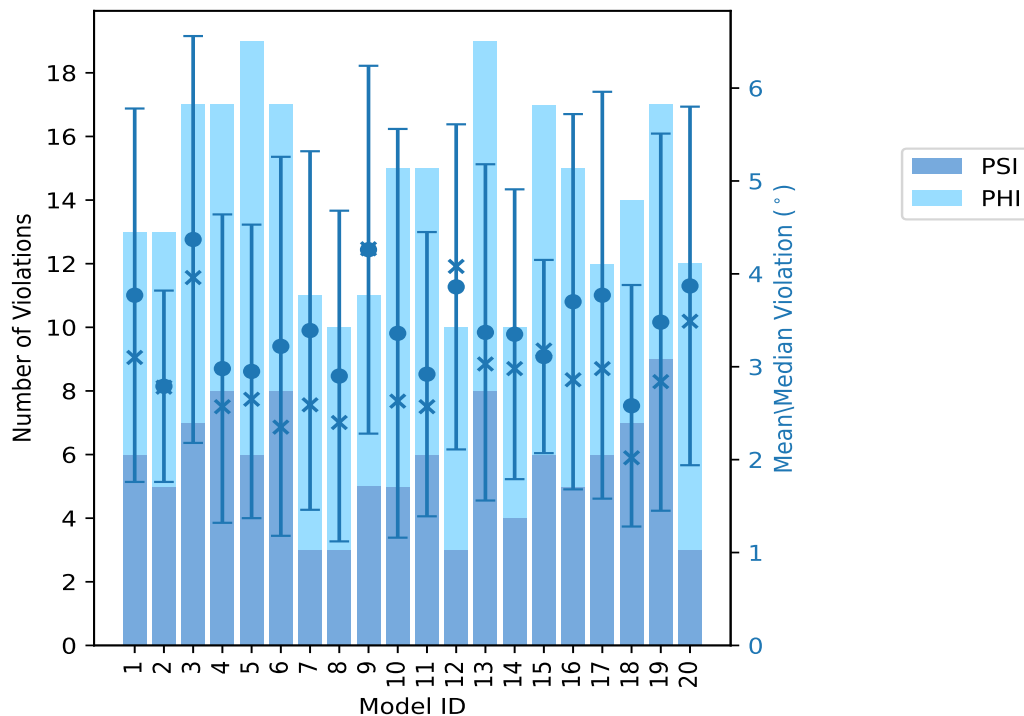
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	6	7	13	3.77	7.53	2.01	3.1
2	5	8	13	2.79	4.37	1.03	2.78
3	7	10	17	4.37	8.89	2.19	3.96
4	8	9	17	2.98	6.42	1.66	2.57
5	6	13	19	2.95	6.58	1.58	2.65
6	8	9	17	3.22	8.06	2.04	2.35
7	3	8	11	3.39	8.21	1.93	2.59
8	3	7	10	2.9	6.4	1.78	2.4
9	5	6	11	4.26	8.35	1.98	4.27
10	5	10	15	3.36	8.46	2.2	2.63
11	6	9	15	2.92	5.9	1.53	2.57
12	3	7	10	3.86	7.41	1.75	4.08
13	8	11	19	3.37	7.36	1.81	3.03
14	4	6	10	3.35	5.99	1.56	2.98
15	6	11	17	3.11	4.89	1.04	3.18
16	5	10	15	3.7	7.82	2.02	2.86
17	6	6	12	3.77	7.87	2.19	2.98
18	7	7	14	2.58	5.54	1.3	2.02
19	9	8	17	3.48	7.81	2.03	2.84
20	3	9	12	3.87	7.71	1.93	3.49

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	Total	Count ¹	%
13	7	20	1	5.0
6	4	10	2	10.0
3	4	7	3	15.0
3	2	5	4	20.0
3	1	4	5	25.0
2	1	3	6	30.0
0	1	1	7	35.0
1	1	2	8	40.0
2	1	3	9	45.0
0	2	2	10	50.0
0	0	0	11	55.0

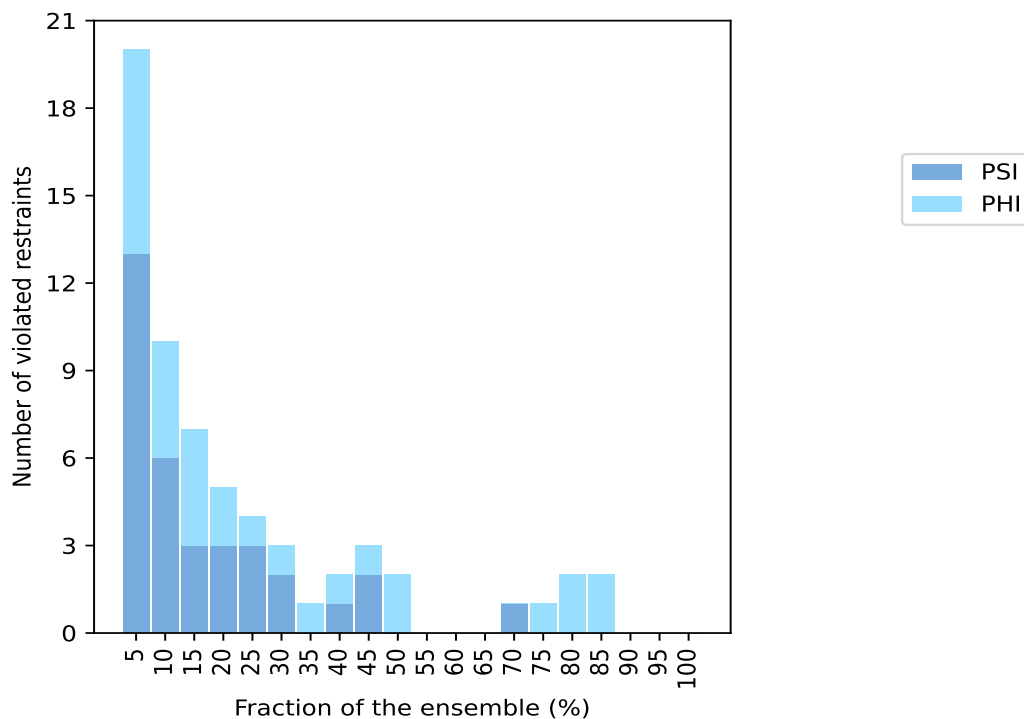
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
1	0	1	14	70.0
0	1	1	15	75.0
0	2	2	16	80.0
0	2	2	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)

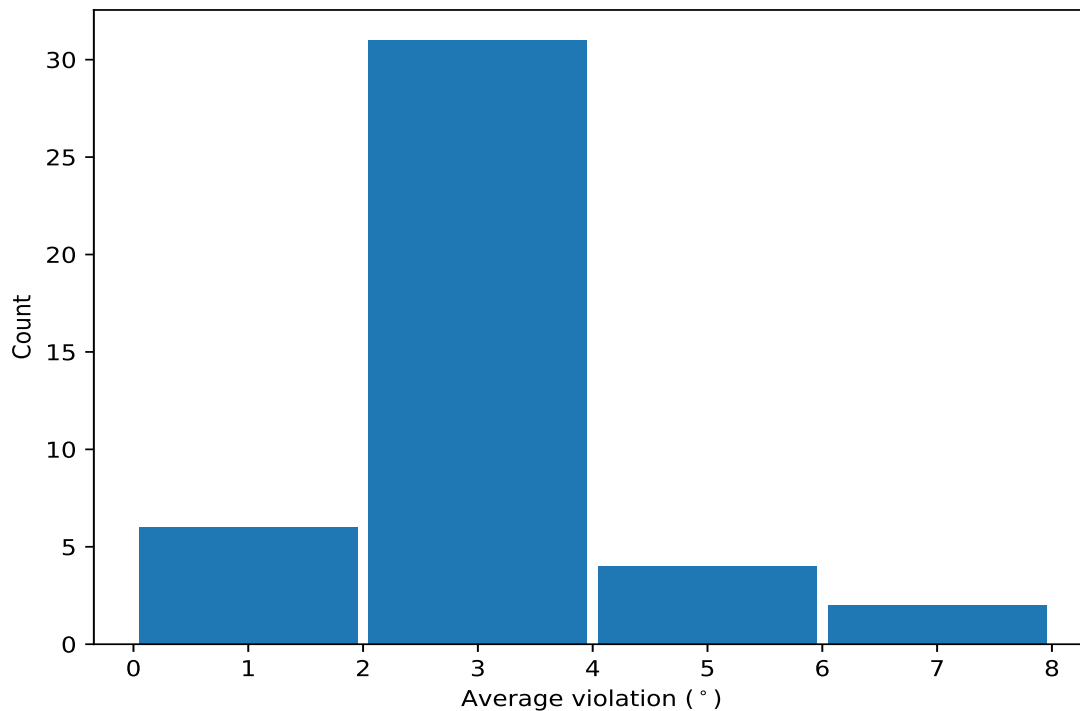


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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 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.

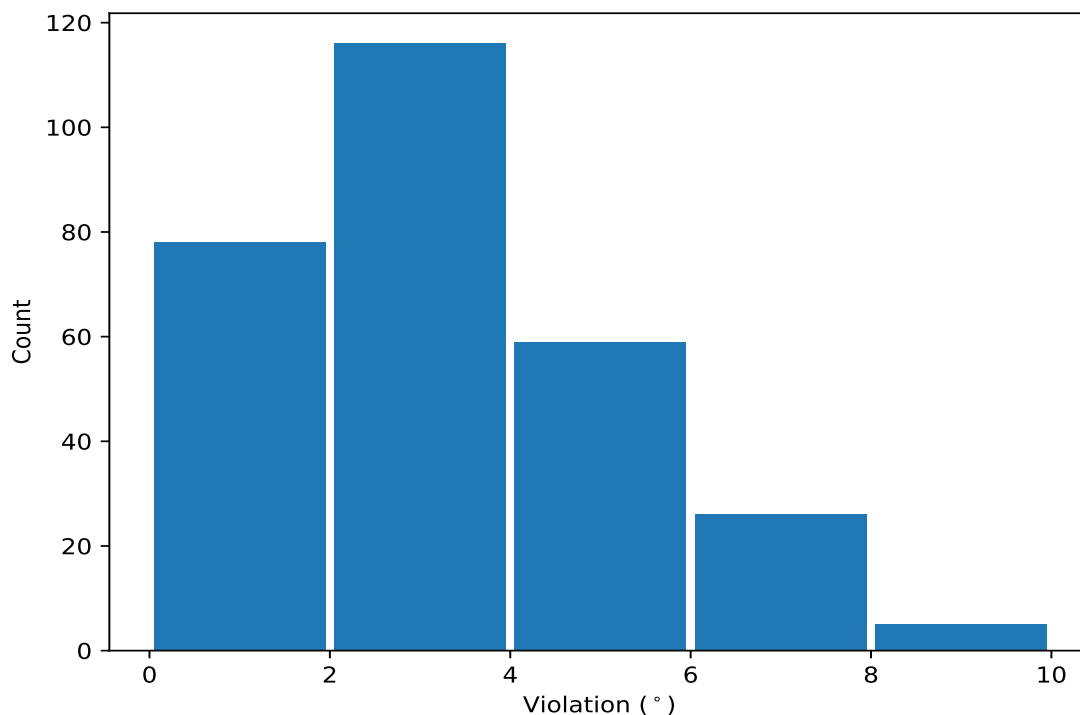
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,95)	1:596:A:ASN:C	1:597:A:LYS:N	1:597:A:LYS:CA	1:597:A:LYS:C	17	3.83	1.83	3.75
(1,89)	1:590:A:SER:C	1:591:A:VAL:N	1:591:A:VAL:CA	1:591:A:VAL:C	17	3.44	1.46	3.1
(1,73)	1:579:A:LYS:C	1:580:A:LYS:N	1:580:A:LYS:CA	1:580:A:LYS:C	16	4.84	1.63	4.98
(1,129)	1:621:A:SER:C	1:622:A:VAL:N	1:622:A:VAL:CA	1:622:A:VAL:C	16	3.77	1.74	3.53
(1,185)	1:651:A:ALA:C	1:652:A:PHE:N	1:652:A:PHE:CA	1:652:A:PHE:C	15	2.81	1.41	2.43
(1,100)	1:599:A:MET:N	1:599:A:MET:CA	1:599:A:MET:C	1:600:A:LYS:N	14	6.04	1.59	6.02
(1,33)	1:553:A:VAL:C	1:554:A:THR:N	1:554:A:THR:CA	1:554:A:THR:C	10	2.54	0.96	2.51
(1,27)	1:550:A:PRO:C	1:551:A:ASN:N	1:551:A:ASN:CA	1:551:A:ASN:C	10	2.28	1.18	1.92
(1,43)	1:558:A:THR:C	1:559:A:LYS:N	1:559:A:LYS:CA	1:559:A:LYS:C	9	3.85	1.27	3.85
(1,90)	1:591:A:VAL:N	1:591:A:VAL:CA	1:591:A:VAL:C	1:592:A:LEU:N	9	2.35	1.05	2.09

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 (°)
(1,67)	1:573:A:ARG:C	1:574:A:GLU:N	1:574:A:GLU:CA	1:574:A:GLU:C	3	8.89
(1,198)	1:662:A:ARG:N	1:662:A:ARG:CA	1:662:A:ARG:C	1:663:A:ILE:N	10	8.46
(1,100)	1:599:A:MET:N	1:599:A:MET:CA	1:599:A:MET:C	1:600:A:LYS:N	9	8.35
(1,100)	1:599:A:MET:N	1:599:A:MET:CA	1:599:A:MET:C	1:600:A:LYS:N	7	8.21
(1,122)	1:618:A:ARG:N	1:618:A:ARG:CA	1:618:A:ARG:C	1:619:A:THR:N	6	8.06
(1,153)	1:633:A:LEU:C	1:634:A:SER:N	1:634:A:SER:CA	1:634:A:SER:C	17	7.87
(1,129)	1:621:A:SER:C	1:622:A:VAL:N	1:622:A:VAL:CA	1:622:A:VAL:C	16	7.82
(1,198)	1:662:A:ARG:N	1:662:A:ARG:CA	1:662:A:ARG:C	1:663:A:ILE:N	19	7.81
(1,121)	1:617:A:ARG:C	1:618:A:ARG:N	1:618:A:ARG:CA	1:618:A:ARG:C	20	7.71
(1,196)	1:660:A:LEU:N	1:660:A:LEU:CA	1:660:A:LEU:C	1:661:A:ASP:N	10	7.67