wwPDB NMR Structure Validation Summary Report

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BMRB ID	:	36490
Title	:	Solution structure of RRM1 of Human SART3
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Deposited on	:	2022-05-29

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:

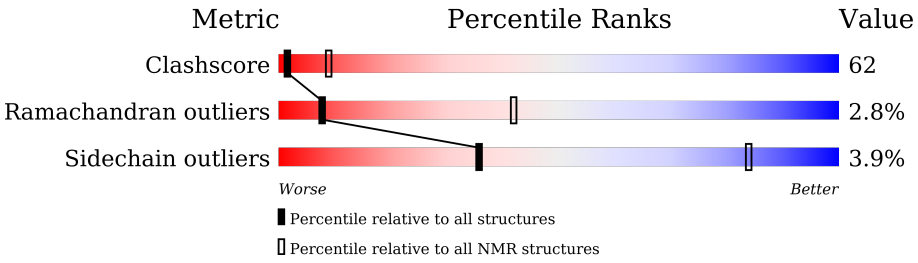
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 84%.

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	94	15% 68% · 12% ·

2 Ensemble composition and analysis

This entry contains 20 models. Model 19 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:701-A:779 (79)	0.62	19

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1426 atoms, of which 705 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Squamous cell carcinoma antigen recognized by T-cells 3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	90	1426	453	705	123	139	6	0

There are 4 discrepancies between the modelled and reference sequences:

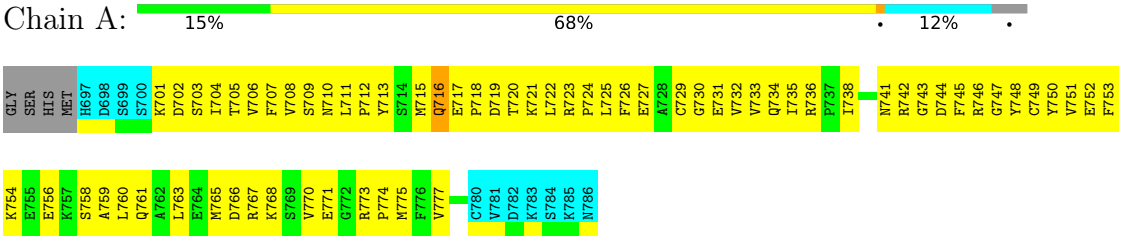
Chain	Residue	Modelled	Actual	Comment	Reference
A	693	GLY	-	expression tag	UNP Q15020
A	694	SER	-	expression tag	UNP Q15020
A	695	HIS	-	expression tag	UNP Q15020
A	696	MET	-	expression tag	UNP Q15020

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.

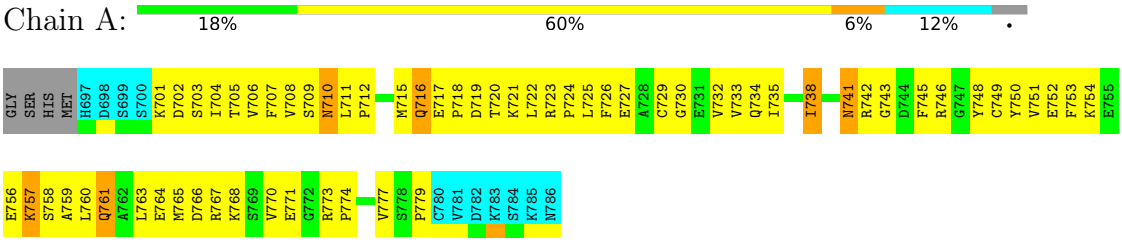
• Molecule 1: Squamous cell carcinoma antigen recognized by T-cells 3



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

The representative model is number 19. Colouring as in section 4.1 above.

• Molecule 1: Squamous cell carcinoma antigen recognized by T-cells 3



5 Refinement protocol and experimental data overview

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

Of the 1000 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
X-PLOR NIH	structure calculation	

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	1115
Number of shifts mapped to atoms	1114
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

6 Model quality

6.1 Standard geometry

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	638	630	630	78±10
All	All	12760	12600	12600	1563

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 62.

5 of 522 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:722:LEU:HD11	1:A:735:ILE:CD1	1.00	1.84	1	11
1:A:726:PHE:CE1	1:A:751:VAL:HG21	0.97	1.93	7	2
1:A:722:LEU:HD13	1:A:726:PHE:CD1	0.96	1.94	14	5
1:A:708:VAL:HG12	1:A:777:VAL:HG22	0.96	1.38	8	9
1:A:722:LEU:HD11	1:A:735:ILE:HD11	0.94	1.39	10	7

6.3 Torsion angles

6.3.1 Protein backbone

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	79/94 (84%)	73±1 (92±1%)	4±1 (5±1%)	2±1 (3±1%)	8 42
All	All	1580/1880 (84%)	1459 (92%)	77 (5%)	44 (3%)	8 42

All 5 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	716	GLN	20
1	A	743	GLY	16
1	A	741	ASN	6
1	A	766	ASP	1
1	A	710	ASN	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	72/86 (84%)	69±1 (96±2%)	3±1 (4±2%)	36 84
All	All	1440/1720 (84%)	1384 (96%)	56 (4%)	36 84

5 of 18 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	760	LEU	20
1	A	723	ARG	7
1	A	754	LYS	7
1	A	750	TYR	3
1	A	738	ILE	3

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 monosaccharides 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

The completeness of assignment taking into account all chemical shift lists is 84% 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: *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	1115
Number of shifts mapped to atoms	1114
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. First 5 (of 1) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	704	ILE	HD12	0.949	0.01	.
1	A	704	ILE	HD13	0.949	0.01	.
1	A	704	ILE	HG22	0.688	0.01	.
1	A	704	ILE	HG23	0.688	0.01	.
1	A	705	THR	HG22	1.337	0.01	.
1	A	705	THR	HG23	1.337	0.01	.
1	A	706	VAL	HG12	0.992	0.01	.
1	A	706	VAL	HG13	0.992	0.01	.
1	A	706	VAL	HG22	0.790	0.01	.
1	A	706	VAL	HG23	0.790	0.01	.
1	A	708	VAL	HG12	1.060	0.01	.
1	A	708	VAL	HG13	1.060	0.01	.
1	A	708	VAL	HG22	0.748	0.01	.
1	A	708	VAL	HG23	0.748	0.01	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	711	LEU	HD12	0.858	0.02	.
1	A	711	LEU	HD13	0.858	0.02	.
1	A	711	LEU	HD22	0.794	0.01	.
1	A	711	LEU	HD23	0.794	0.01	.
1	A	715	MET	HE2	1.934	0.02	.
1	A	715	MET	HE3	1.934	0.02	.
1	A	720	THR	HG22	1.225	0.00	.
1	A	720	THR	HG23	1.225	0.00	.
1	A	722	LEU	HD12	0.880	0.01	.
1	A	722	LEU	HD13	0.880	0.01	.
1	A	722	LEU	HD22	0.815	0.01	.
1	A	722	LEU	HD23	0.815	0.01	.
1	A	725	LEU	HD12	0.800	0.01	.
1	A	725	LEU	HD13	0.800	0.01	.
1	A	725	LEU	HD22	0.649	0.01	.
1	A	725	LEU	HD23	0.649	0.01	.
1	A	728	ALA	HB2	1.489	0.01	.
1	A	728	ALA	HB3	1.489	0.01	.
1	A	732	VAL	HG12	0.781	0.01	.
1	A	732	VAL	HG13	0.781	0.01	.
1	A	732	VAL	HG22	0.461	0.01	.
1	A	732	VAL	HG23	0.461	0.01	.
1	A	733	VAL	HG12	0.850	0.01	.
1	A	733	VAL	HG13	0.850	0.01	.
1	A	735	ILE	HD12	0.810	0.01	.
1	A	735	ILE	HD13	0.810	0.01	.
1	A	735	ILE	HG22	0.640	0.01	.
1	A	735	ILE	HG23	0.640	0.01	.
1	A	738	ILE	HG22	0.867	0.01	.
1	A	738	ILE	HG23	0.867	0.01	.
1	A	751	VAL	HG12	0.001	0.01	.
1	A	751	VAL	HG13	0.001	0.01	.
1	A	751	VAL	HG22	-0.128	0.01	.
1	A	751	VAL	HG23	-0.128	0.01	.
1	A	759	ALA	HB2	1.370	0.01	.
1	A	759	ALA	HB3	1.370	0.01	.
1	A	760	LEU	HD12	0.900	0.01	.
1	A	760	LEU	HD13	0.900	0.01	.
1	A	760	LEU	HD22	0.882	0.00	.
1	A	760	LEU	HD23	0.882	0.00	.
1	A	762	ALA	HB2	1.713	0.01	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	762	ALA	HB3	1.713	0.01	.
1	A	763	LEU	HD12	1.033	0.01	.
1	A	763	LEU	HD13	1.033	0.01	.
1	A	763	LEU	HD22	0.750	0.01	.
1	A	763	LEU	HD23	0.750	0.01	.
1	A	765	MET	HE2	1.773	0.01	.
1	A	765	MET	HE3	1.773	0.01	.
1	A	770	VAL	HG12	0.847	0.01	.
1	A	770	VAL	HG13	0.847	0.01	.
1	A	770	VAL	HG22	0.793	0.02	.
1	A	770	VAL	HG23	0.793	0.02	.
1	A	775	MET	HE2	1.523	0.00	.
1	A	775	MET	HE3	1.523	0.00	.
1	A	777	VAL	HG12	1.114	0.01	.
1	A	777	VAL	HG13	1.114	0.01	.
1	A	777	VAL	HG22	0.986	0.01	.
1	A	777	VAL	HG23	0.986	0.01	.
1	A	781	VAL	HG12	0.852	0.01	.
1	A	781	VAL	HG13	0.852	0.01	.

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	697	HIS	HB3	3.024	0.01	.

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	88	-0.31 ± 0.26	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	85	0.27 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	84	0.11 ± 0.22	None needed (< 0.5 ppm)
^{15}N	81	0.55 ± 0.47	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 84%, i.e. 928 atoms were assigned a chemical shift out of a possible 1099. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	373/387 (96%)	152/156 (97%)	150/158 (95%)	71/73 (97%)
Sidechain	516/625 (83%)	347/403 (86%)	164/194 (85%)	5/28 (18%)
Aromatic	39/87 (45%)	28/42 (67%)	11/45 (24%)	0/0 (—%)
Overall	928/1099 (84%)	527/601 (88%)	325/397 (82%)	76/101 (75%)

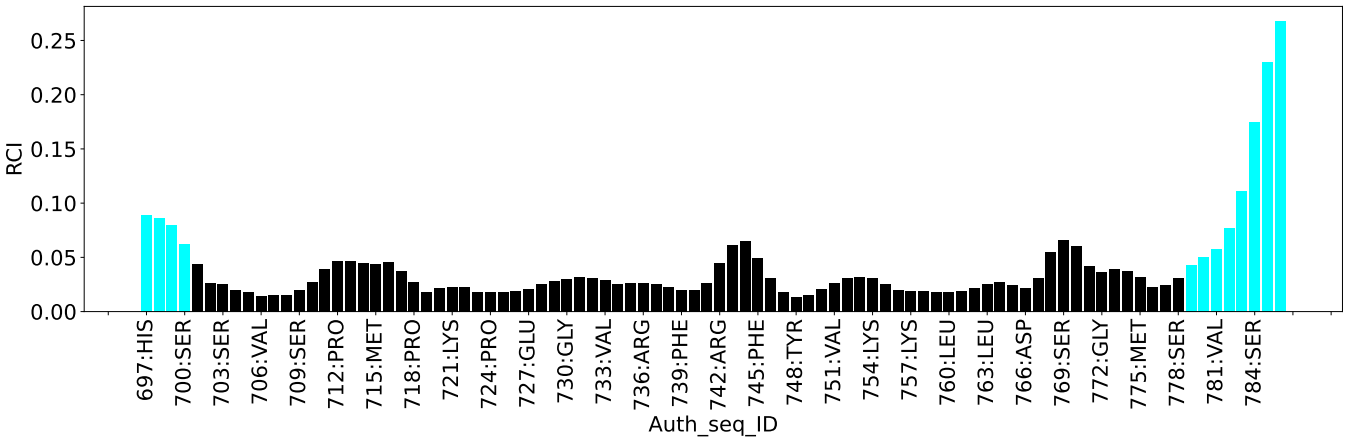
7.1.4 Statistically unusual chemical shifts

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:



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	1401
Intra-residue (|i-j|=0)	321
Sequential (|i-j|=1)	422
Medium range (|i-j|>1 and |i-j|<5)	227
Long range (|i-j|≥5)	431
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	184
Number of unmapped restraints	0
Number of restraints per residue	16.9
Number of long range restraints per residue[1]	4.6

[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)	7.8	0.2
0.2-0.5 (Medium)	3.3	0.46
>0.5 (Large)	0.9	0.77

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)	6.5	3.63
10.0-20.0 (Medium)	None	None
>20.0 (Large)	1.0	89.26

9 Distance violation analysis (i)

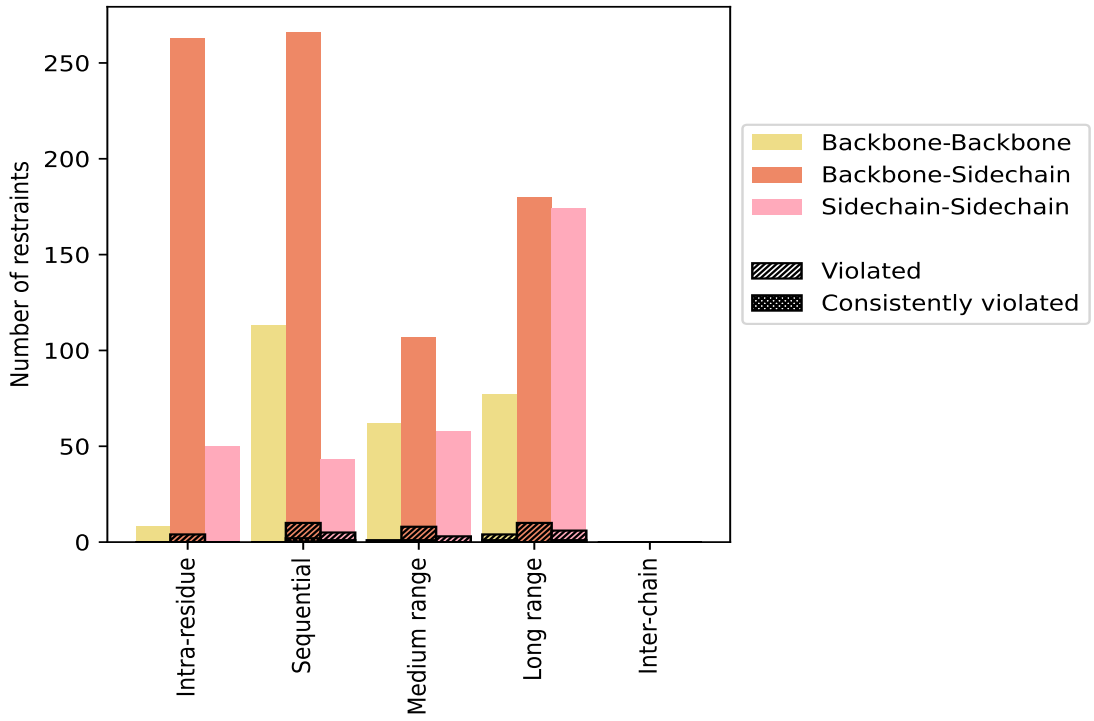
9.1 Summary of distance violations (i)

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)	321	22.9	4	1.2	0.3	0	0.0	0.0
Backbone-Backbone	8	0.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	263	18.8	4	1.5	0.3	0	0.0	0.0
Sidechain-Sidechain	50	3.6	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	422	30.1	15	3.6	1.1	3	0.7	0.2
Backbone-Backbone	113	8.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	266	19.0	10	3.8	0.7	2	0.8	0.1
Sidechain-Sidechain	43	3.1	5	11.6	0.4	1	2.3	0.1
Medium range (|i-j|>1 & |i-j|<5)	227	16.2	12	5.3	0.9	1	0.4	0.1
Backbone-Backbone	62	4.4	1	1.6	0.1	0	0.0	0.0
Backbone-Sidechain	107	7.6	8	7.5	0.6	1	0.9	0.1
Sidechain-Sidechain	58	4.1	3	5.2	0.2	0	0.0	0.0
Long range (|i-j|≥5)	431	30.8	20	4.6	1.4	2	0.5	0.1
Backbone-Backbone	77	5.5	4	5.2	0.3	1	1.3	0.1
Backbone-Sidechain	180	12.8	10	5.6	0.7	0	0.0	0.0
Sidechain-Sidechain	174	12.4	6	3.4	0.4	1	0.6	0.1
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	1401	100.0	51	3.6	3.6	6	0.4	0.4
Backbone-Backbone	260	18.6	5	1.9	0.4	1	0.4	0.1
Backbone-Sidechain	816	58.2	32	3.9	2.3	3	0.4	0.2
Sidechain-Sidechain	325	23.2	14	4.3	1.0	2	0.6	0.1

[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	1	6	2	5	0	14	0.24	0.72	0.16	0.19
2	1	4	3	3	0	11	0.19	0.39	0.09	0.17
3	2	7	2	4	0	15	0.22	0.71	0.15	0.18
4	0	4	4	4	0	12	0.22	0.73	0.17	0.16
5	1	6	3	5	0	15	0.23	0.72	0.16	0.16
6	0	4	2	3	0	9	0.25	0.73	0.19	0.17
7	1	5	3	5	0	14	0.21	0.7	0.15	0.16
8	0	6	2	4	0	12	0.24	0.73	0.17	0.18
9	1	6	2	5	0	14	0.23	0.73	0.16	0.18
10	1	5	3	5	0	14	0.21	0.7	0.16	0.14
11	1	7	3	4	0	15	0.23	0.74	0.16	0.18

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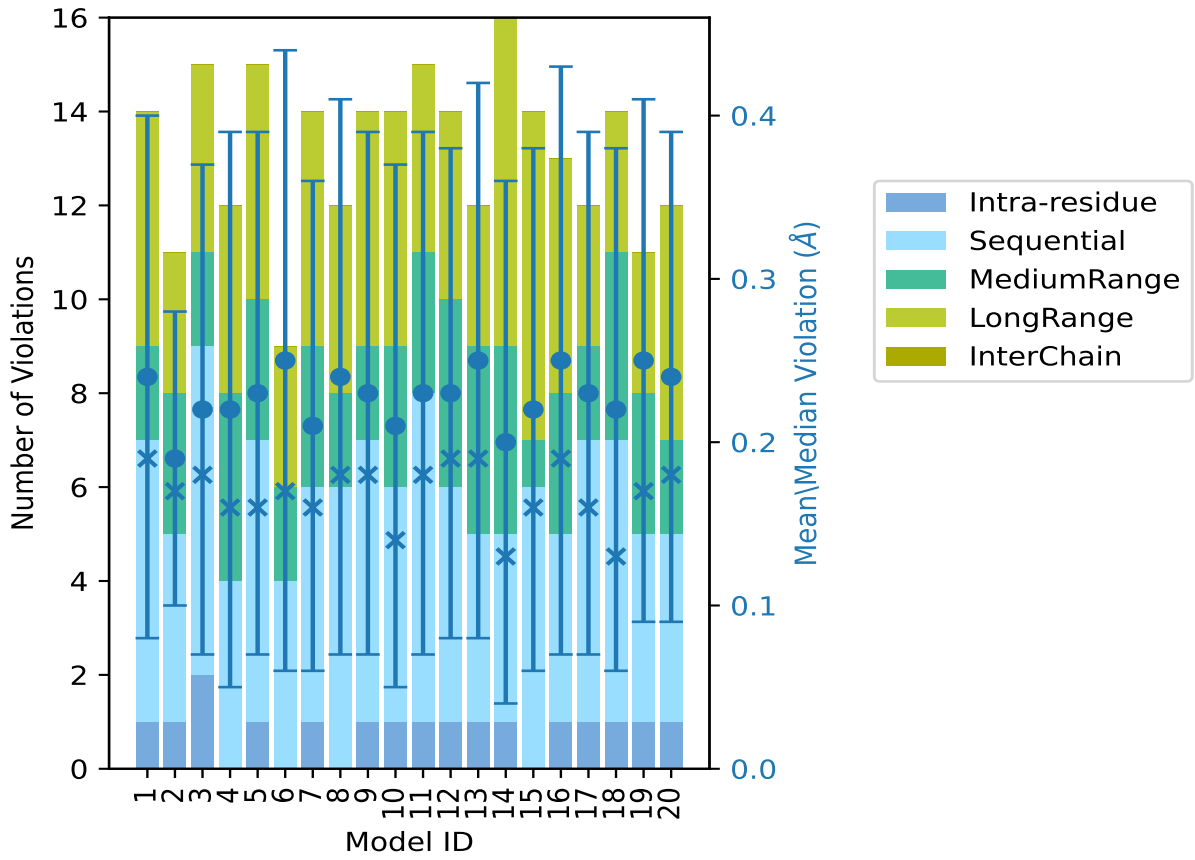
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	1	5	4	4	0	14	0.23	0.66	0.15	0.19
13	1	4	4	3	0	12	0.25	0.72	0.17	0.19
14	1	4	4	7	0	16	0.2	0.72	0.16	0.13
15	0	6	1	7	0	14	0.22	0.72	0.16	0.16
16	1	4	3	5	0	13	0.25	0.77	0.18	0.19
17	1	6	2	3	0	12	0.23	0.7	0.16	0.16
18	1	6	4	3	0	14	0.22	0.67	0.16	0.13
19	1	4	3	3	0	11	0.25	0.7	0.16	0.17
20	1	4	2	5	0	12	0.24	0.68	0.15	0.18

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

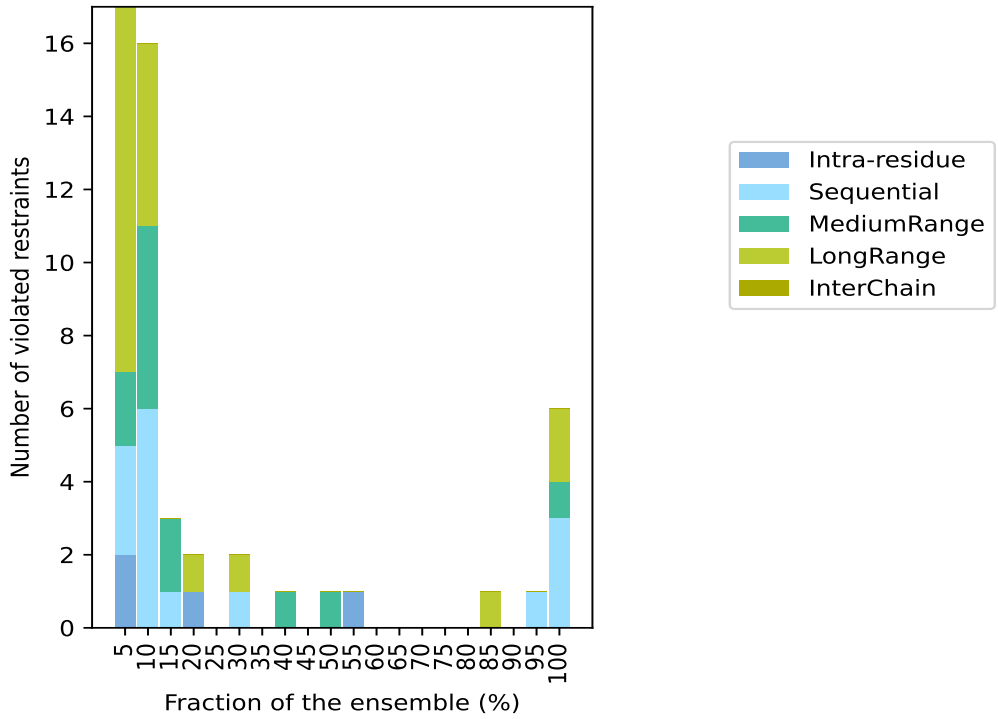
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1350(IR:317, SQ:407, MR:215, LR:411, IC:0) restraints are not violated in the ensemble.

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

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

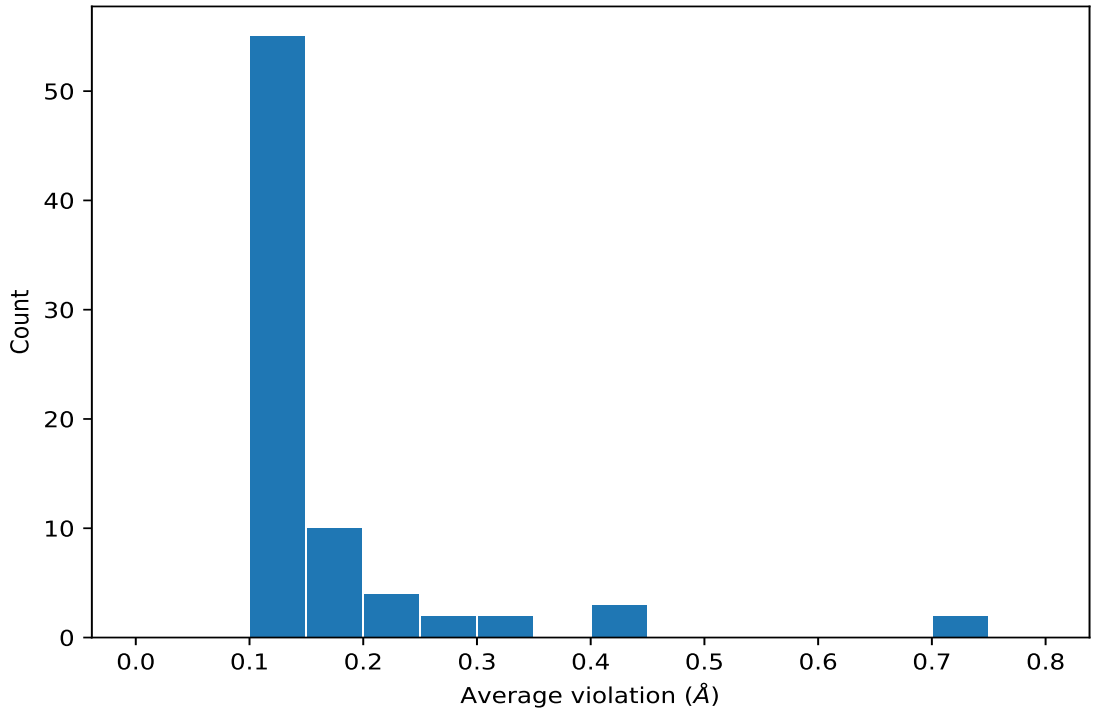
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,103)	1:705:A:THR:HG21	1:707:A:PHE:H	20	0.4	0.02	0.4
(1,103)	1:705:A:THR:HG22	1:707:A:PHE:H	20	0.4	0.02	0.4
(1,103)	1:705:A:THR:HG23	1:707:A:PHE:H	20	0.4	0.02	0.4
(1,1136)	1:763:A:LEU:HG	1:764:A:GLU:HG2	20	0.26	0.02	0.26
(1,1136)	1:763:A:LEU:HG	1:764:A:GLU:HG3	20	0.26	0.02	0.26
(1,481)	1:723:A:ARG:HD2	1:728:A:ALA:HB1	20	0.19	0.08	0.16
(1,481)	1:723:A:ARG:HD2	1:728:A:ALA:HB2	20	0.19	0.08	0.16
(1,481)	1:723:A:ARG:HD2	1:728:A:ALA:HB3	20	0.19	0.08	0.16
(1,907)	1:751:A:VAL:HA	1:752:A:GLU:HG2	20	0.18	0.01	0.19
(1,907)	1:751:A:VAL:HA	1:752:A:GLU:HG3	20	0.18	0.01	0.19
(1,1286)	1:771:A:GLU:HB2	1:772:A:GLY:HA2	20	0.17	0.02	0.16
(1,645)	1:731:A:GLU:H	1:753:A:PHE:HA	20	0.15	0.03	0.14
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG2	19	0.71	0.02	0.72
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG3	19	0.71	0.02	0.72
(1,406)	1:719:A:ASP:HA	1:735:A:ILE:H	17	0.14	0.03	0.13
(1,473)	1:723:A:ARG:H	1:723:A:ARG:HD3	11	0.31	0.03	0.31

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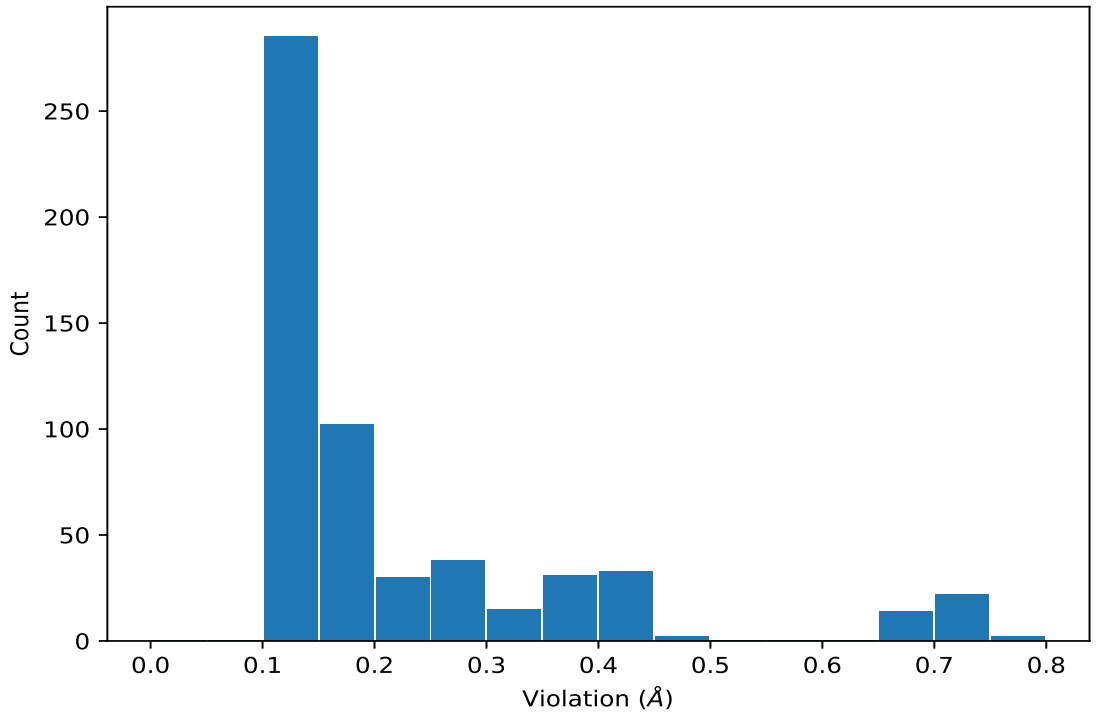
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,775)	1:735:A:ILE:H	1:737:A:PRO:HD2	10	0.11	0.01	0.11

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

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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



9.5.2 Table : All distance violations

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)
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG2	16	0.77
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG3	16	0.77
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG2	11	0.74
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG3	11	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG2	4	0.73
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG3	4	0.73
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG2	6	0.73
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG3	6	0.73
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG2	8	0.73
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG3	8	0.73
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG2	9	0.73
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG3	9	0.73
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG2	1	0.72
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG3	1	0.72
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG2	5	0.72
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG3	5	0.72
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG2	13	0.72
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG3	13	0.72
(1,542)	1:726:A:PHE:H	1:727:A:GLU:HG2	14	0.72

10 Dihedral-angle violation analysis

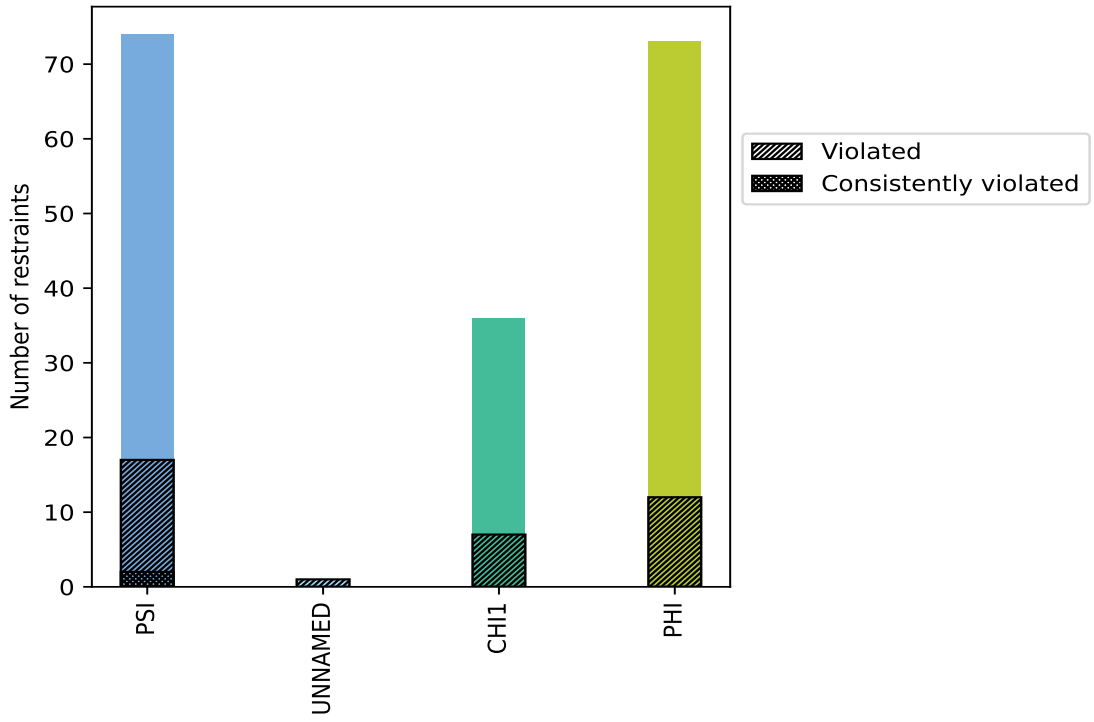
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	74	40.2	17	23.0	9.2	2	2.7	1.1
UNNAMED	1	0.5	1	100.0	0.5	0	0.0	0.0
CHI1	36	19.6	7	19.4	3.8	0	0.0	0.0
PHI	73	39.7	12	16.4	6.5	0	0.0	0.0
Total	184	100.0	37	20.1	20.1	2	1.1	1.1

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



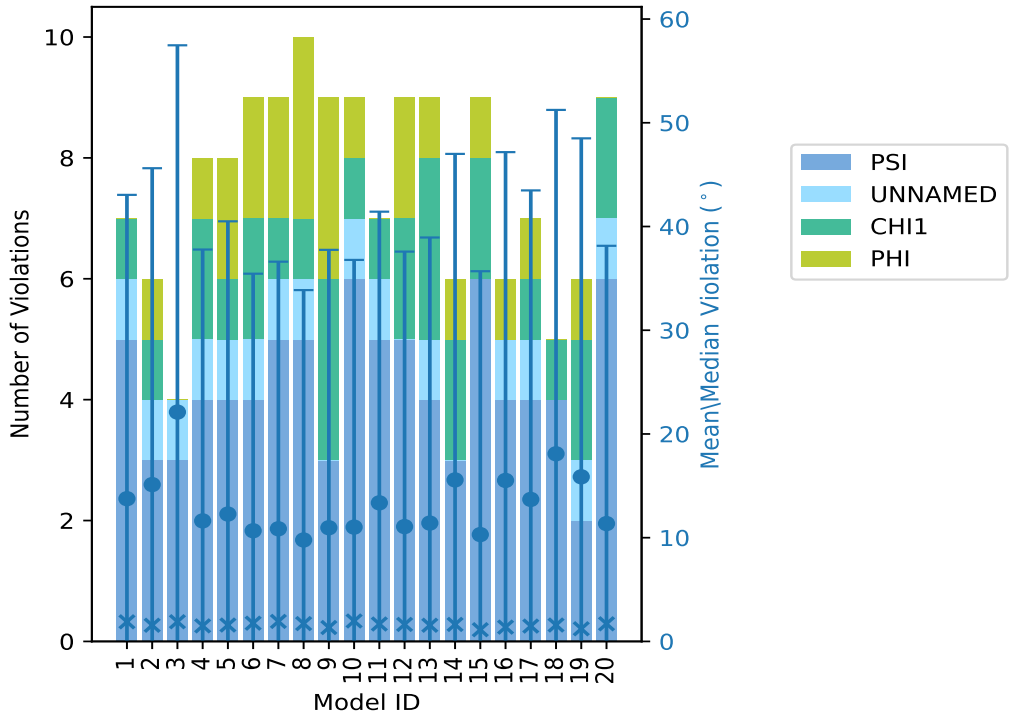
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations					Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	UNNAMED	CHI1	PHI	Total				
1	5	1	1	0	7	13.76	85.49	29.29	1.89
2	3	1	1	1	6	15.12	83.33	30.5	1.56
3	3	1	0	0	4	22.11	83.36	35.36	1.9
4	4	1	2	1	8	11.62	80.82	26.16	1.5
5	4	1	1	2	8	12.28	86.94	28.22	1.58
6	4	1	2	2	9	10.67	80.73	24.78	1.76
7	5	1	1	2	9	10.86	83.68	25.75	1.93
8	5	1	1	3	10	9.78	82.03	24.09	1.72
9	3	0	3	3	9	10.96	86.74	26.79	1.34
10	6	1	1	1	9	11.02	83.86	25.76	1.97
11	5	1	1	0	7	13.36	82.1	28.07	1.68
12	5	0	2	2	9	11.07	86.05	26.51	1.64
13	4	1	3	1	9	11.41	89.26	27.53	1.56
14	3	0	2	1	6	15.57	85.84	31.43	1.64
15	6	0	2	1	9	10.3	82.09	25.39	1.13
16	4	1	0	1	6	15.52	86.28	31.65	1.38
17	4	1	1	1	7	13.69	86.65	29.79	1.48
18	4	0	1	0	5	18.09	84.39	33.15	1.58
19	2	1	2	1	6	15.87	88.84	32.63	1.22
20	6	1	2	0	9	11.36	87.11	26.78	1.7

10.2.1 Bar graph : Dihedral violation statistics for each model



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

10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints					Fraction of the ensemble	
PSI	UNNAMED	CHI1	PHI	Total	Count[1]	%
3	0	3	7	13	1	5.0
5	0	1	0	6	2	10.0
3	0	0	4	7	3	15.0
1	0	1	1	3	4	20.0
2	0	0	0	2	5	25.0
0	0	0	0	0	6	30.0
0	0	0	0	0	7	35.0
0	0	0	0	0	8	40.0
1	0	1	0	2	9	45.0
0	0	0	0	0	10	50.0
0	0	1	0	1	11	55.0

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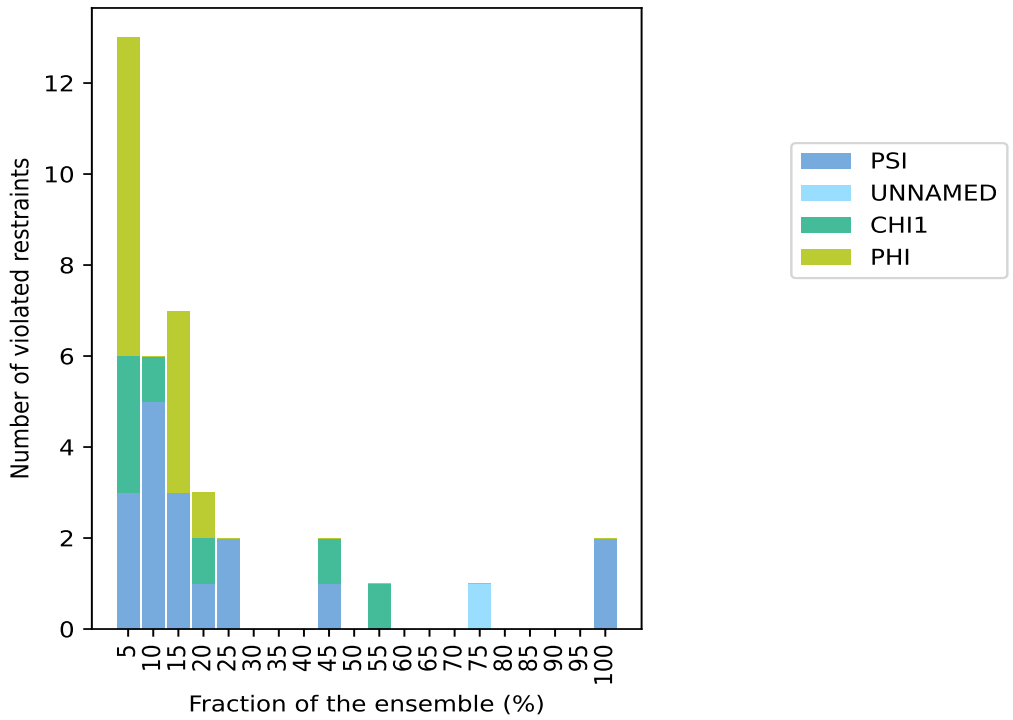
Number of violated restraints					Fraction of the ensemble	
PSI	UNNAMED	CHI1	PHI	Total	Count[1]	%
0	0	0	0	0	12	60.0
0	0	0	0	0	13	65.0
0	0	0	0	0	14	70.0
0	1	0	0	1	15	75.0
0	0	0	0	0	16	80.0
0	0	0	0	0	17	85.0
0	0	0	0	0	18	90.0
0	0	0	0	0	19	95.0
2	0	0	0	2	20	100.0

[1] Number of models with violations

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

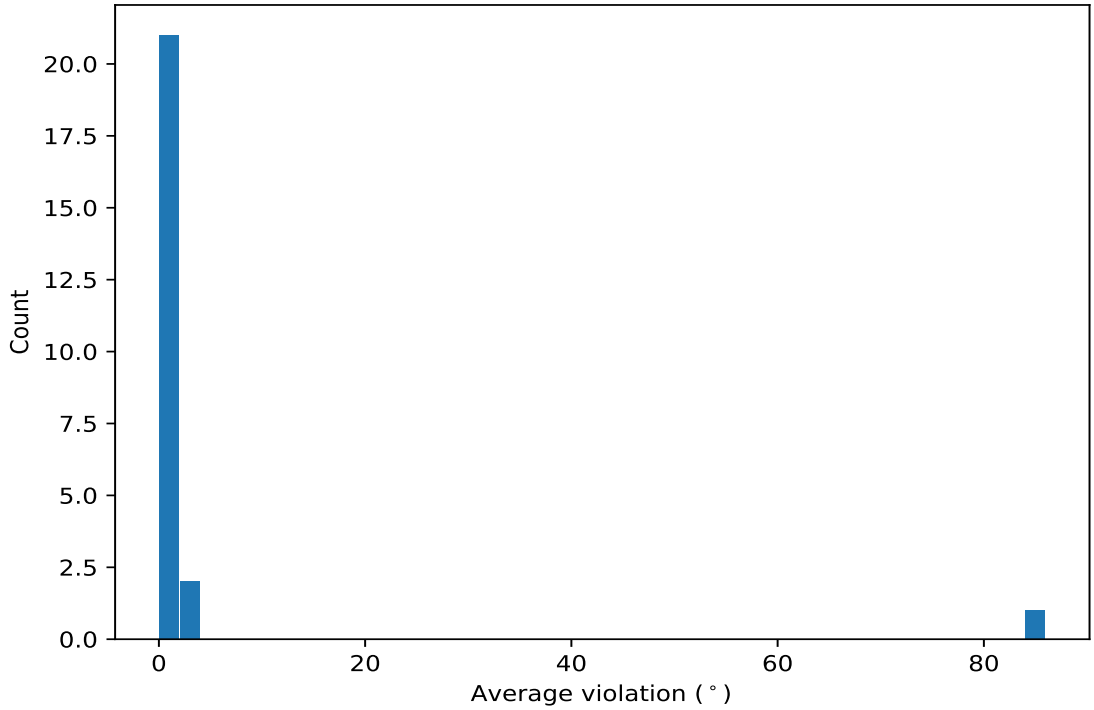


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

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

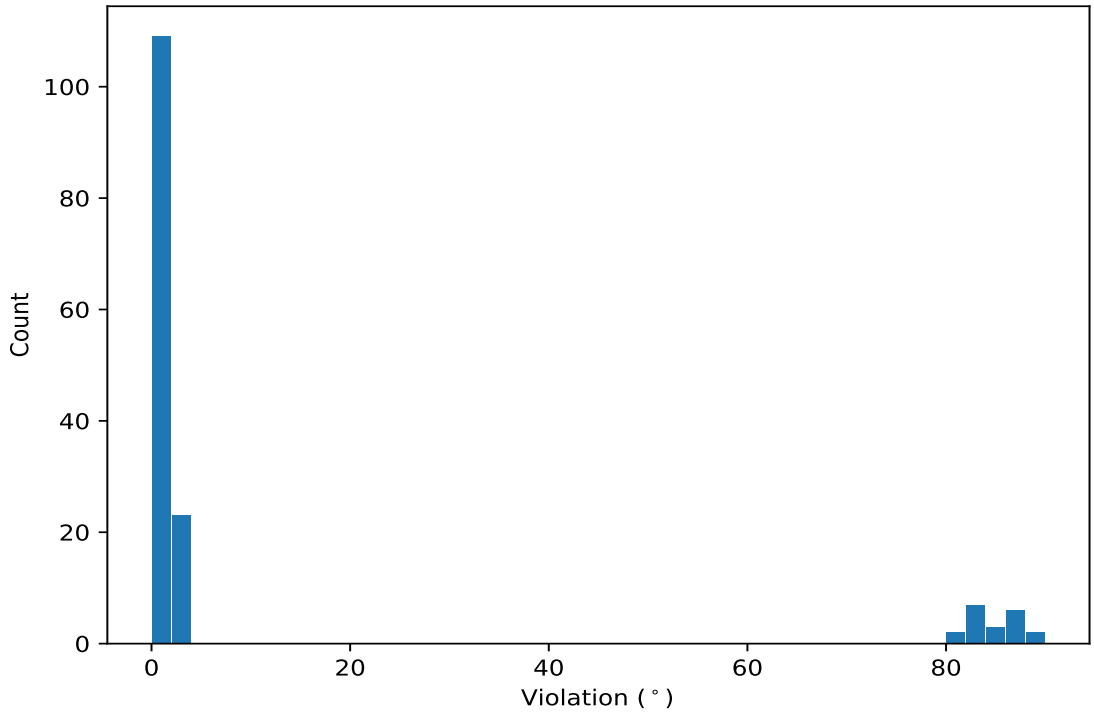
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Media
(1,147)	1:768:A:LYS:N	1:768:A:LYS:CA	1:768:A:LYS:C	1:769:A:SER:N	20	84.78	2.45	84.94
(1,14)	1:706:A:VAL:N	1:706:A:VAL:CA	1:706:A:VAL:C	1:707:A:PHE:N	20	1.81	0.38	1.79
(1,151)	1:705:A:THR:N	1:705:A:THR:CA	1:705:A:THR:CB	1:705:A:THR:CG2	15	1.75	0.65	1.52
(1,161)	1:725:A:LEU:N	1:725:A:LEU:CA	1:725:A:LEU:CB	1:725:A:LEU:CG	11	1.31	0.13	1.31
(1,176)	1:767:A:ARG:N	1:767:A:ARG:CA	1:767:A:ARG:CB	1:767:A:ARG:CG	9	1.57	0.49	1.54
(1,67)	1:736:A:ARG:N	1:736:A:ARG:CA	1:736:A:ARG:C	1:737:A:PRO:N	9	1.36	0.18	1.32
(1,27)	1:715:A:MET:N	1:715:A:MET:CA	1:715:A:MET:C	1:716:A:GLN:N	5	2.04	0.74	1.68
(1,20)	1:709:A:SER:N	1:709:A:SER:CA	1:709:A:SER:C	1:710:A:ASN:N	5	1.45	0.28	1.35
(1,18)	1:708:A:VAL:N	1:708:A:VAL:CA	1:708:A:VAL:C	1:709:A:SER:N	4	1.7	0.53	1.66
(1,34)	1:719:A:ASP:C	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	4	1.7	0.16	1.67

[1] Number of violated models, [2]Standard 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 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 (°)
(1,147)	1:768:A:LYS:N	1:768:A:LYS:CA	1:768:A:LYS:C	1:769:A:SER:N	13	89.26
(1,147)	1:768:A:LYS:N	1:768:A:LYS:CA	1:768:A:LYS:C	1:769:A:SER:N	19	88.84
(1,147)	1:768:A:LYS:N	1:768:A:LYS:CA	1:768:A:LYS:C	1:769:A:SER:N	20	87.11
(1,147)	1:768:A:LYS:N	1:768:A:LYS:CA	1:768:A:LYS:C	1:769:A:SER:N	5	86.94
(1,147)	1:768:A:LYS:N	1:768:A:LYS:CA	1:768:A:LYS:C	1:769:A:SER:N	9	86.74
(1,147)	1:768:A:LYS:N	1:768:A:LYS:CA	1:768:A:LYS:C	1:769:A:SER:N	17	86.65
(1,147)	1:768:A:LYS:N	1:768:A:LYS:CA	1:768:A:LYS:C	1:769:A:SER:N	16	86.28
(1,147)	1:768:A:LYS:N	1:768:A:LYS:CA	1:768:A:LYS:C	1:769:A:SER:N	12	86.05
(1,147)	1:768:A:LYS:N	1:768:A:LYS:CA	1:768:A:LYS:C	1:769:A:SER:N	14	85.84
(1,147)	1:768:A:LYS:N	1:768:A:LYS:CA	1:768:A:LYS:C	1:769:A:SER:N	1	85.49