wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID	:	8IEX
BMRB ID	:	36548
Title	:	Solution structure of AtWRKY11-DBD
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Deposited on	:	2023-02-16

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

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

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

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

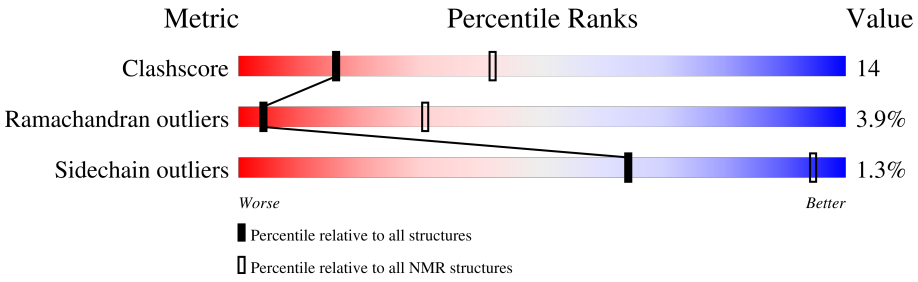
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 69%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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

Mol	Chain	Length	Quality of chain
1	A	94	47% 15% • 31% 6%

2 Ensemble composition and analysis

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:228-A:233, A:250-A:302 (59)	0.59	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 4 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1433 atoms, of which 718 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Probable WRKY transcription factor 11.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	88	1432	446	718	139	124	5	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	MET	-	initiating methionine	UNP Q9SV15
A	309	LEU	-	expression tag	UNP Q9SV15
A	310	GLU	-	expression tag	UNP Q9SV15
A	311	HIS	-	expression tag	UNP Q9SV15
A	312	HIS	-	expression tag	UNP Q9SV15
A	313	HIS	-	expression tag	UNP Q9SV15
A	314	HIS	-	expression tag	UNP Q9SV15
A	315	HIS	-	expression tag	UNP Q9SV15

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	1	1	1

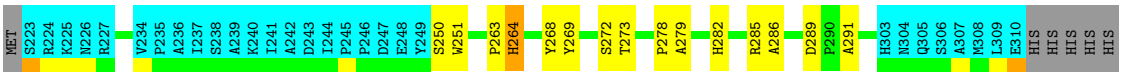
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Probable WRKY transcription factor 11

Chain A:

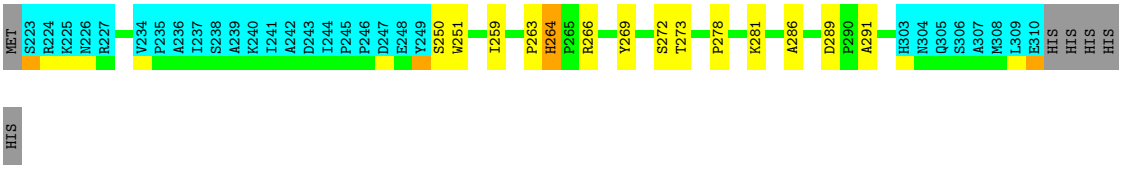


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 5. Colouring as in section 4.1 above.

- Molecule 1: Probable WRKY transcription factor 11

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 216 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The authors did not provide any information on software used for structure solution, optimization or 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	895
Number of shifts mapped to atoms	895
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	69%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.59±0.00	0±0/502 (0.0± 0.0%)	0.92±0.00	1±0/674 (0.1± 0.0%)
All	All	0.59	0/10040 (0.0%)	0.92	20/13480 (0.1%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	269	TYR	CB-CG-CD1	-6.31	117.21	121.00	4	20

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	487	492	490	14±3
All	All	9760	9840	9800	276

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 14.

5 of 107 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:270:LYS:NZ	1:A:280:ARG:HE	0.88	1.65	10	1
1:A:270:LYS:NZ	1:A:280:ARG:NH2	0.67	2.43	20	1
1:A:278:PRO:O	1:A:279:ALA:CB	0.64	2.45	8	11
1:A:263:PRO:O	1:A:264:HIS:CG	0.63	2.52	16	13
1:A:253:LYS:NZ	1:A:256:GLN:NE2	0.63	2.46	15	3

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	59/94 (63%)	55±1 (93±2%)	2±1 (3±2%)	2±1 (4±1%)	4	31
All	All	1180/1880 (63%)	1098 (93%)	36 (3%)	46 (4%)	4	31

All 4 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	264	HIS	19
1	A	279	ALA	13
1	A	273	THR	11
1	A	250	SER	3

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	51/82 (62%)	50±1 (99±2%)	1±1 (1±2%)	64	94
All	All	1020/1640 (62%)	1007 (99%)	13 (1%)	64	94

5 of 8 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	273	THR	3
1	A	264	HIS	2
1	A	277	CYS	2
1	A	250	SER	2
1	A	251	TRP	1

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 oligosaccharides 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 69% for the well-defined parts and 67% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *wk11_CS*

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	895
Number of shifts mapped to atoms	895
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

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

- Chemical shift has been reported more than once. First 5 (of 0) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	231	THR	HG22	1.13420	.	.
1	A	231	THR	HG23	1.13420	.	.
1	A	232	VAL	HG12	1.03862	.	.
1	A	232	VAL	HG13	1.03862	.	.
1	A	232	VAL	HG22	1.05183	.	.
1	A	232	VAL	HG23	1.05183	.	.
1	A	234	VAL	HG12	0.82927	.	.
1	A	234	VAL	HG13	0.82927	.	.
1	A	234	VAL	HG22	0.95103	.	.
1	A	234	VAL	HG23	0.95103	.	.
1	A	236	ALA	HB2	1.26715	.	.
1	A	236	ALA	HB3	1.26715	.	.
1	A	237	ILE	HG22	0.90775	.	.
1	A	237	ILE	HG23	0.90775	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	239	ALA	HB2	1.39333	.	.
1	A	239	ALA	HB3	1.39333	.	.
1	A	241	ILE	HD12	0.89751	.	.
1	A	241	ILE	HD13	0.89751	.	.
1	A	241	ILE	HG22	0.59508	.	.
1	A	241	ILE	HG23	0.59508	.	.
1	A	242	ALA	HB2	1.44778	.	.
1	A	242	ALA	HB3	1.44778	.	.
1	A	244	ILE	HD12	-0.03942	.	.
1	A	244	ILE	HD13	-0.03942	.	.
1	A	244	ILE	HG22	0.73786	.	.
1	A	244	ILE	HG23	0.73786	.	.
1	A	259	ILE	HD12	0.84626	.	.
1	A	259	ILE	HD13	0.84626	.	.
1	A	259	ILE	HG22	0.89746	.	.
1	A	259	ILE	HG23	0.89746	.	.
1	A	273	THR	HG22	1.14090	.	.
1	A	273	THR	HG23	1.14090	.	.
1	A	279	ALA	HB2	0.59154	.	.
1	A	279	ALA	HB3	0.59154	.	.
1	A	283	VAL	HG12	0.64392	.	.
1	A	283	VAL	HG13	0.64392	.	.
1	A	283	VAL	HG22	0.86695	.	.
1	A	283	VAL	HG23	0.86695	.	.
1	A	286	ALA	HB2	1.50275	.	.
1	A	286	ALA	HB3	1.50275	.	.
1	A	287	LEU	HD12	0.93542	.	.
1	A	287	LEU	HD13	0.93542	.	.
1	A	287	LEU	HD22	1.00353	.	.
1	A	287	LEU	HD23	1.00353	.	.
1	A	291	ALA	HB2	1.48455	.	.
1	A	291	ALA	HB3	1.48455	.	.
1	A	293	LEU	HD12	0.71197	.	.
1	A	293	LEU	HD13	0.71197	.	.
1	A	293	LEU	HD22	0.76095	.	.
1	A	293	LEU	HD23	0.76095	.	.
1	A	294	ILE	HD12	0.87194	.	.
1	A	294	ILE	HD13	0.87194	.	.
1	A	294	ILE	HG22	0.76527	.	.
1	A	294	ILE	HG23	0.76527	.	.
1	A	295	VAL	HG12	0.12956	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	295	VAL	HG13	0.12956	.	.
1	A	295	VAL	HG22	0.73595	.	.
1	A	295	VAL	HG23	0.73595	.	.
1	A	296	THR	HG22	0.93573	.	.
1	A	296	THR	HG23	0.93573	.	.
1	A	309	LEU	HD12	0.86111	.	.
1	A	309	LEU	HD13	0.86111	.	.
1	A	309	LEU	HD22	0.92003	.	.
1	A	309	LEU	HD23	0.92003	.	.

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	83	-0.02 ± 0.16	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	79	0.05 ± 0.16	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	79	-0.68 ± 0.41	None needed (imprecise)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 69%, i.e. 585 atoms were assigned a chemical shift out of a possible 851. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	230/290 (79%)	118/118 (100%)	58/118 (49%)	54/54 (100%)
Sidechain	318/480 (66%)	199/308 (65%)	119/141 (84%)	0/31 (0%)
Aromatic	37/81 (46%)	23/39 (59%)	14/36 (39%)	0/6 (0%)
Overall	585/851 (69%)	340/465 (73%)	191/295 (65%)	54/91 (59%)

7.1.4 Statistically unusual chemical shifts (i)

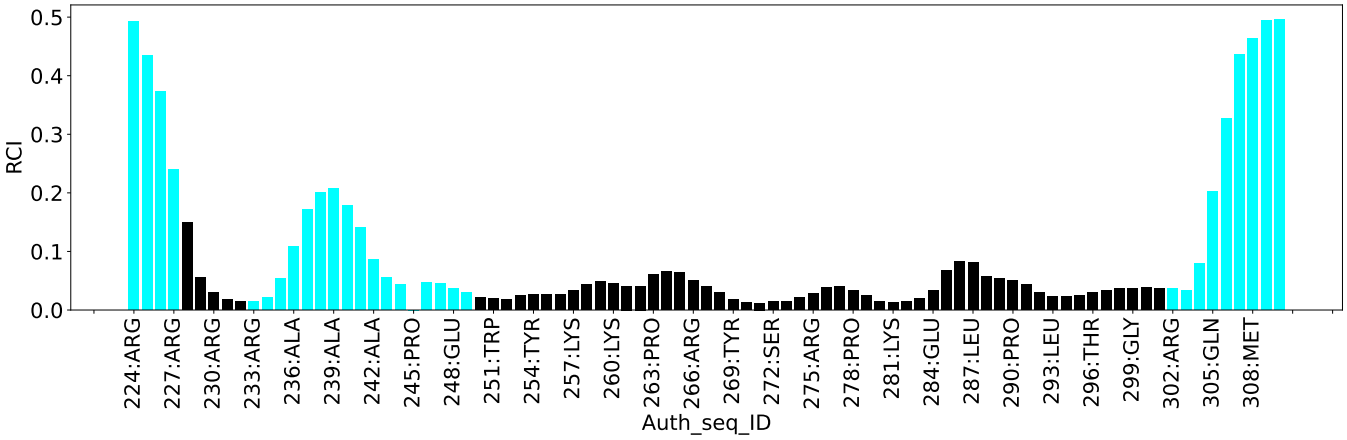
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	281	LYS	HE3	0.31	1.92 – 3.89	-13.2
1	A	281	LYS	HE2	1.07	1.95 – 3.88	-9.5
1	A	281	LYS	HD3	-0.06	0.54 – 2.65	-7.8
1	A	281	LYS	HD2	0.06	0.58 – 2.64	-7.5
1	A	281	LYS	HG2	0.03	0.13 – 2.61	-5.4
1	A	281	LYS	HG3	-0.01	0.04 – 2.67	-5.2

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	911
Intra-residue (|i-j|=0)	474
Sequential (|i-j|=1)	235
Medium range (|i-j|>1 and |i-j|<5)	40
Long range (|i-j|≥5)	162
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	120
Number of unmapped restraints	0
Number of restraints per residue	10.9
Number of long range restraints per residue[1]	1.7

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å
are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	40.1	0.2
0.2-0.5 (Medium)	48.0	0.49
>0.5 (Large)	0.7	4.75

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)	10.8	4.74
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

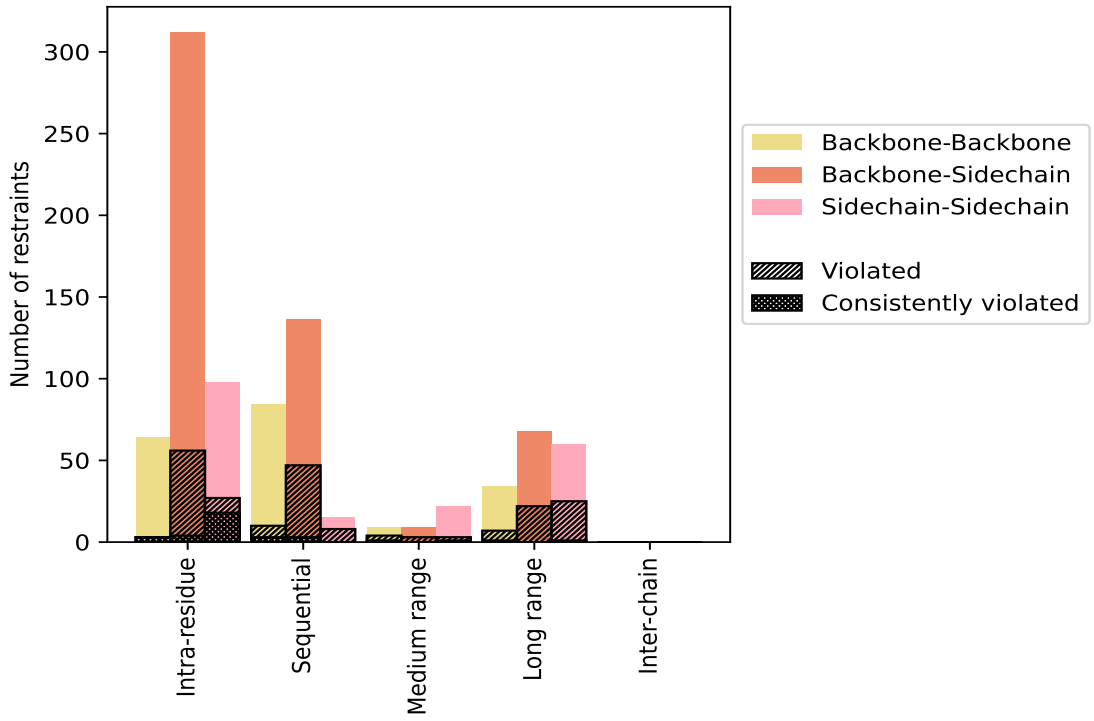
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	474	52.0	86	18.1	9.4	25	5.3	2.7
Backbone-Backbone	64	7.0	3	4.7	0.3	3	4.7	0.3
Backbone-Sidechain	312	34.2	56	17.9	6.1	4	1.3	0.4
Sidechain-Sidechain	98	10.8	27	27.6	3.0	18	18.4	2.0
Sequential (|i-j|=1)	235	25.8	65	27.7	7.1	6	2.6	0.7
Backbone-Backbone	84	9.2	10	11.9	1.1	3	3.6	0.3
Backbone-Sidechain	136	14.9	47	34.6	5.2	3	2.2	0.3
Sidechain-Sidechain	15	1.6	8	53.3	0.9	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	40	4.4	10	25.0	1.1	2	5.0	0.2
Backbone-Backbone	9	1.0	4	44.4	0.4	1	11.1	0.1
Backbone-Sidechain	9	1.0	3	33.3	0.3	0	0.0	0.0
Sidechain-Sidechain	22	2.4	3	13.6	0.3	1	4.5	0.1
Long range (|i-j|≥5)	162	17.8	54	33.3	5.9	2	1.2	0.2
Backbone-Backbone	34	3.7	7	20.6	0.8	1	2.9	0.1
Backbone-Sidechain	68	7.5	22	32.4	2.4	0	0.0	0.0
Sidechain-Sidechain	60	6.6	25	41.7	2.7	1	1.7	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	911	100.0	215	23.6	23.6	35	3.8	3.8
Backbone-Backbone	191	21.0	24	12.6	2.6	8	4.2	0.9
Backbone-Sidechain	525	57.6	128	24.4	14.1	7	1.3	0.8
Sidechain-Sidechain	195	21.4	63	32.3	6.9	20	10.3	2.2

[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	46	21	5	14	0	86	0.24	0.48	0.11	0.22
2	42	23	6	15	0	86	0.25	1.79	0.2	0.2
3	45	27	9	19	0	100	0.25	1.84	0.2	0.22
4	50	26	7	19	0	102	0.24	0.89	0.13	0.2
5	50	26	5	13	0	94	0.26	2.19	0.23	0.22
6	40	30	6	22	0	98	0.23	0.48	0.11	0.22
7	38	25	4	25	0	92	0.24	1.36	0.16	0.2
8	49	18	4	8	0	79	0.25	0.45	0.11	0.24
9	43	23	5	20	0	91	0.23	0.53	0.11	0.2
10	48	25	5	15	0	93	0.25	1.17	0.15	0.21

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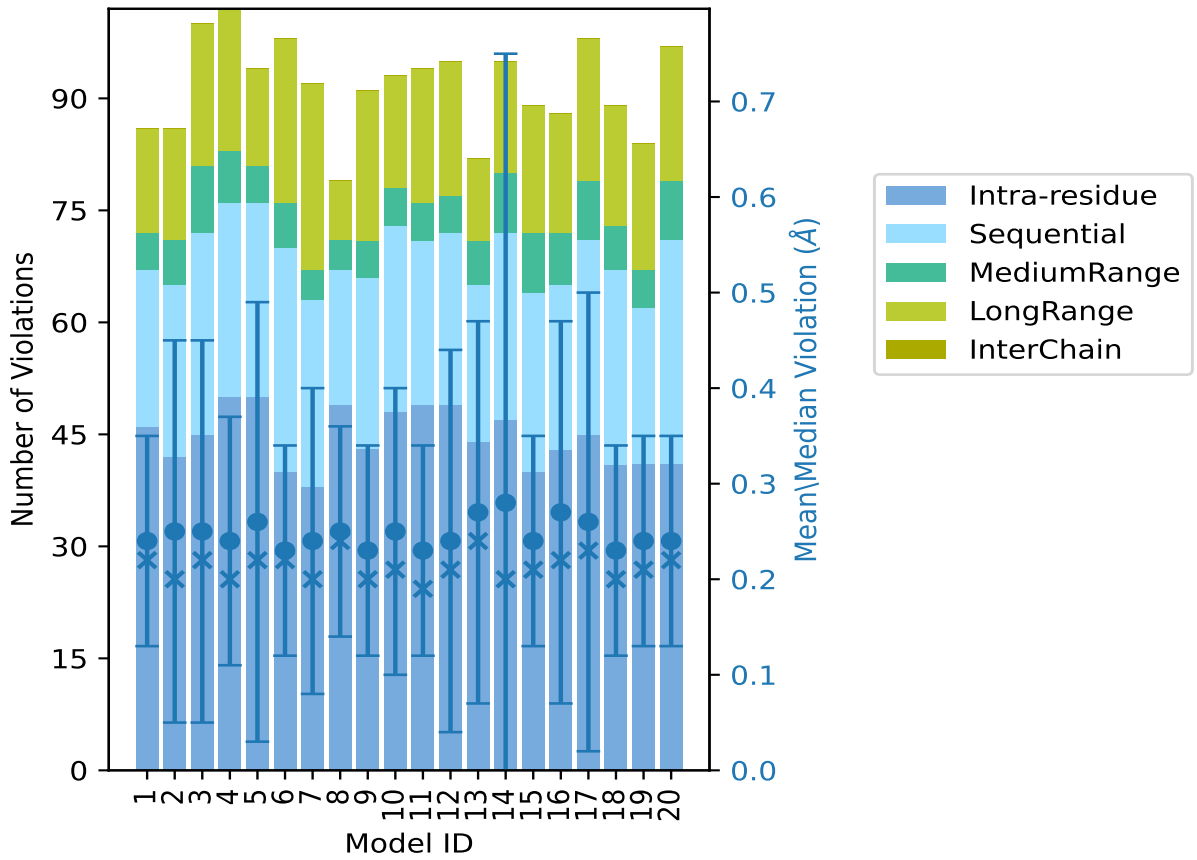
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	49	22	5	18	0	94	0.23	0.45	0.11	0.19
12	49	23	5	18	0	95	0.24	1.84	0.2	0.21
13	44	21	6	11	0	82	0.27	1.81	0.2	0.24
14	47	25	8	15	0	95	0.28	4.75	0.47	0.2
15	40	24	8	17	0	89	0.24	0.47	0.11	0.21
16	43	22	7	16	0	88	0.27	1.84	0.2	0.22
17	45	26	8	19	0	98	0.26	2.35	0.24	0.23
18	41	26	6	16	0	89	0.23	0.48	0.11	0.2
19	41	21	5	17	0	84	0.24	0.45	0.11	0.21
20	41	30	8	18	0	97	0.24	0.49	0.11	0.22

[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

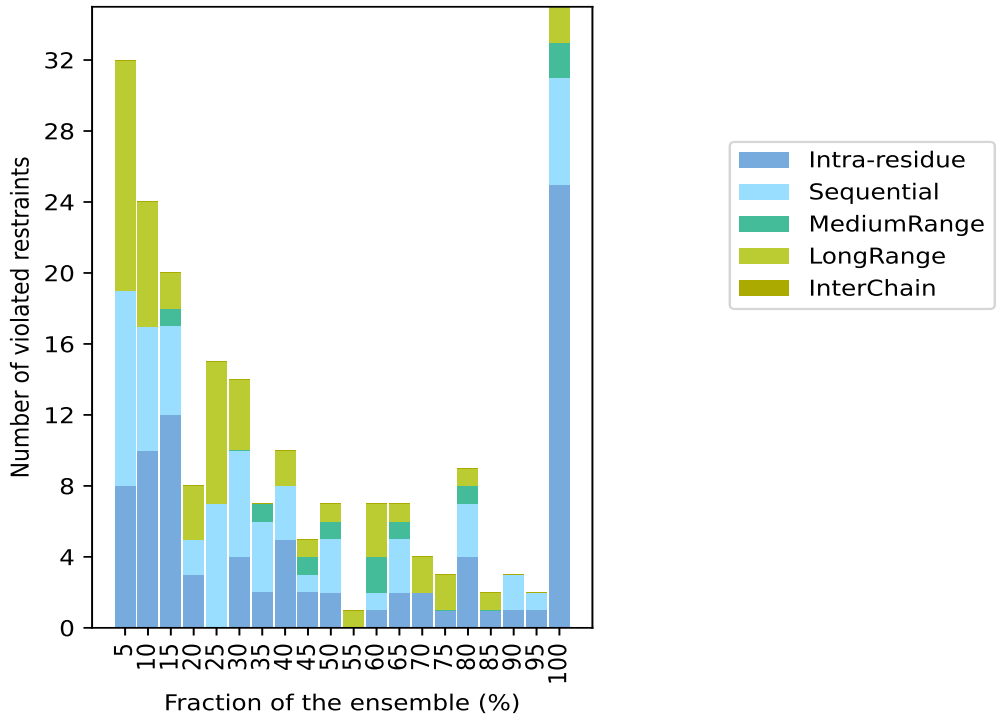
9.3 Distance violation statistics for the ensemble (i)

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, 696(IR:388, SQ:170, MR:30, LR:108, 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]	%
8	11	0	13	0	32	1	5.0
10	7	0	7	0	24	2	10.0
12	5	1	2	0	20	3	15.0
3	2	0	3	0	8	4	20.0
0	7	0	8	0	15	5	25.0
4	6	0	4	0	14	6	30.0
2	4	1	0	0	7	7	35.0
5	3	0	2	0	10	8	40.0
2	1	1	1	0	5	9	45.0
2	3	1	1	0	7	10	50.0
0	0	0	1	0	1	11	55.0
1	1	2	3	0	7	12	60.0
2	3	1	1	0	7	13	65.0
2	0	0	2	0	4	14	70.0
1	0	0	2	0	3	15	75.0
4	3	1	1	0	9	16	80.0
1	0	0	1	0	2	17	85.0
1	2	0	0	0	3	18	90.0
1	1	0	0	0	2	19	95.0
25	6	2	2	0	35	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

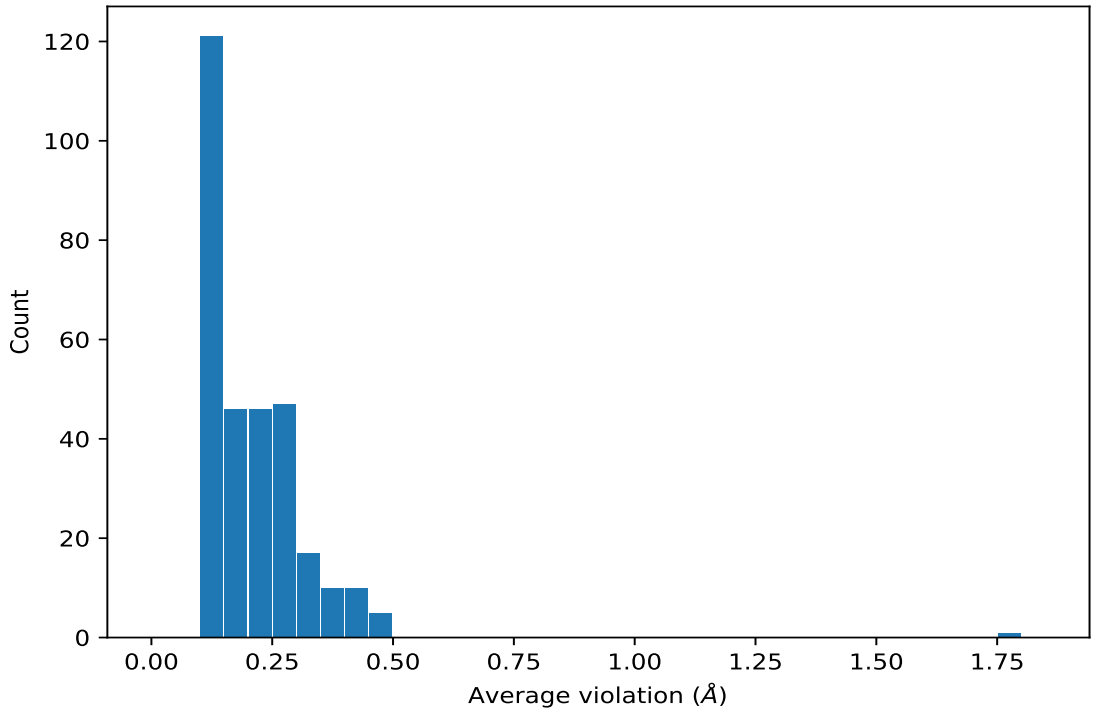
9.3.1 Bar graph : Distance violation statistics for the ensemble



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.

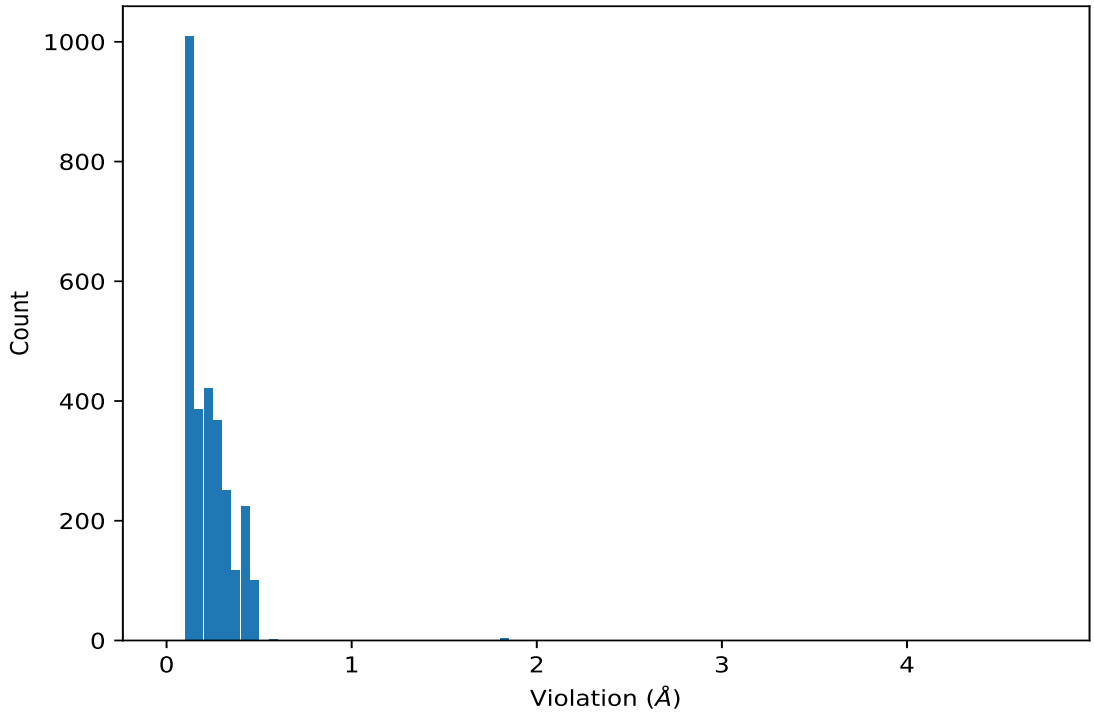
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,177)	1:268:A:TYR:HB3	1:268:A:TYR:HB2	20	0.45	0.0	0.45
(1,175)	1:267:A:GLY:HA3	1:267:A:GLY:HA2	20	0.45	0.0	0.45
(1,639)	1:283:A:VAL:HG11	1:281:A:LYS:HE3	20	0.44	0.04	0.46
(1,639)	1:283:A:VAL:HG12	1:281:A:LYS:HE3	20	0.44	0.04	0.46
(1,639)	1:283:A:VAL:HG13	1:281:A:LYS:HE3	20	0.44	0.04	0.46
(1,186)	1:271:A:CYS:HB3	1:271:A:CYS:HB2	20	0.44	0.0	0.44
(1,504)	1:293:A:LEU:HB3	1:293:A:LEU:HB2	20	0.44	0.0	0.44
(1,112)	1:247:A:ASP:HB3	1:247:A:ASP:HB2	20	0.44	0.0	0.44
(1,418)	1:281:A:LYS:HE3	1:281:A:LYS:HE2	20	0.44	0.0	0.44
(1,581)	1:266:A:ARG:HG2	1:266:A:ARG:HG3	20	0.44	0.0	0.44
(1,582)	1:266:A:ARG:HD2	1:266:A:ARG:HD3	20	0.44	0.0	0.44
(1,658)	1:294:A:ILE:H	1:293:A:LEU:HD11	20	0.39	0.05	0.4

[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)
(1,528)	1:303:A:HIS:HD2	1:274:A:PHE:HB2	14	4.75
(1,528)	1:303:A:HIS:HD2	1:274:A:PHE:HB2	17	2.35
(1,528)	1:303:A:HIS:HD2	1:274:A:PHE:HB2	5	2.19
(1,528)	1:303:A:HIS:HD2	1:274:A:PHE:HB2	3	1.84
(1,528)	1:303:A:HIS:HD2	1:274:A:PHE:HB2	12	1.84
(1,528)	1:303:A:HIS:HD2	1:274:A:PHE:HB2	16	1.84
(1,528)	1:303:A:HIS:HD2	1:274:A:PHE:HB2	13	1.81
(1,528)	1:303:A:HIS:HD2	1:274:A:PHE:HB2	2	1.79
(1,528)	1:303:A:HIS:HD2	1:274:A:PHE:HB2	7	1.36
(1,528)	1:303:A:HIS:HD2	1:274:A:PHE:HB2	10	1.17

10 Dihedral-angle violation analysis

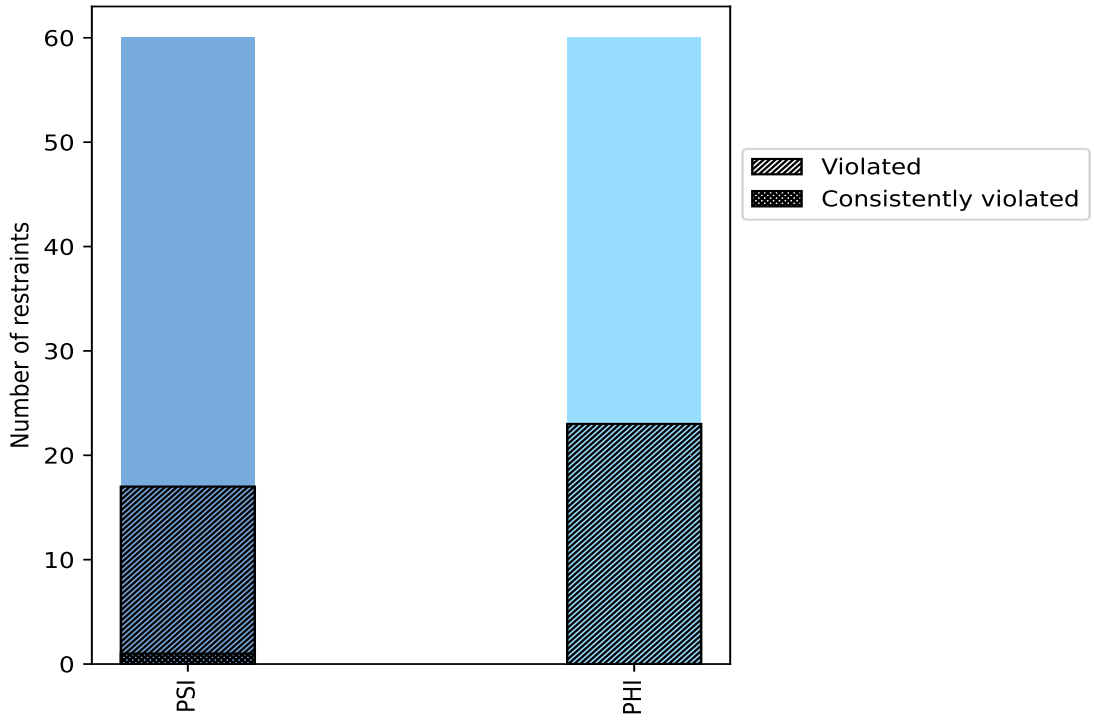
10.1 Summary of dihedral-angle violations

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	60	50.0	17	28.3	14.2	1	1.7	0.8
PHI	60	50.0	23	38.3	19.2	0	0.0	0.0
Total	120	100.0	40	33.3	33.3	1	0.8	0.8

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



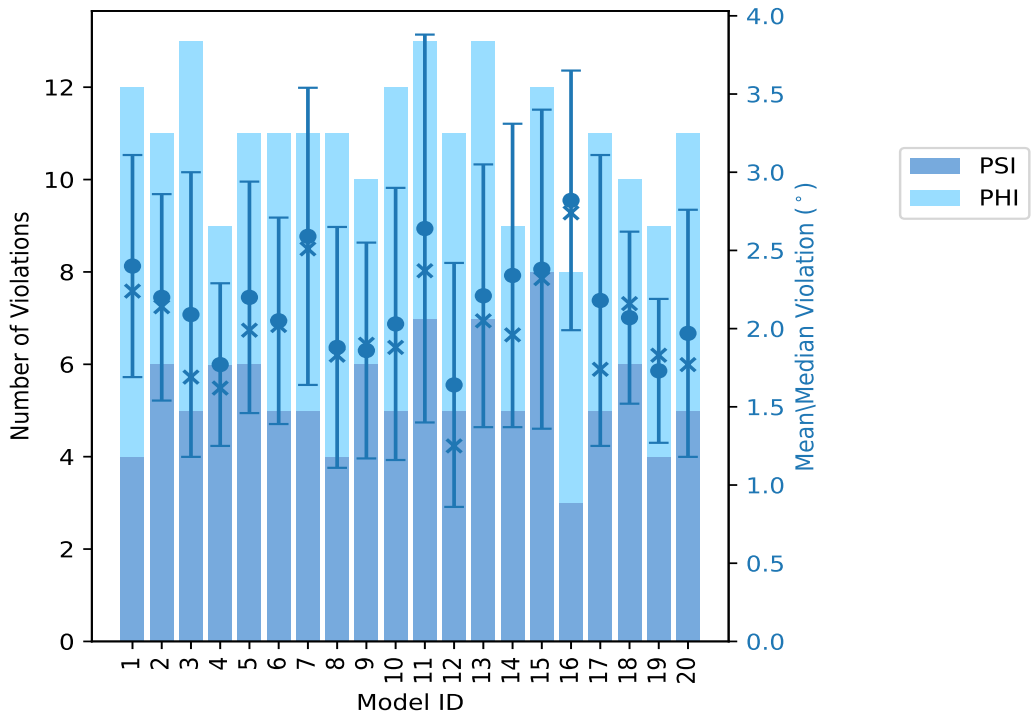
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	4	8	12	2.4	3.57	0.71	2.24
2	6	5	11	2.2	3.14	0.66	2.14
3	5	8	13	2.09	4.34	0.91	1.69
4	6	3	9	1.77	2.84	0.52	1.62
5	6	5	11	2.2	3.41	0.74	1.99
6	5	6	11	2.05	3.07	0.66	2.02
7	5	6	11	2.59	4.36	0.95	2.51
8	4	7	11	1.88	4.02	0.77	1.83
9	6	4	10	1.86	3.09	0.69	1.9
10	5	7	12	2.03	4.44	0.87	1.88
11	7	6	13	2.64	4.74	1.24	2.37
12	5	6	11	1.64	3.66	0.78	1.25
13	7	6	13	2.21	3.79	0.84	2.05
14	5	4	9	2.34	4.18	0.97	1.96
15	8	4	12	2.38	4.68	1.02	2.32
16	3	5	8	2.82	4.3	0.83	2.74
17	5	6	11	2.18	4.07	0.93	1.74
18	6	4	10	2.07	2.82	0.55	2.16
19	4	5	9	1.73	2.57	0.46	1.83
20	5	6	11	1.97	4.13	0.79	1.77

10.2.1 Bar graph : Dihedral violation statistics for each model



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

10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
4	8	12	1	5.0
2	4	6	2	10.0
1	2	3	3	15.0
3	0	3	4	20.0
2	1	3	5	25.0
1	1	2	6	30.0
0	1	1	7	35.0
0	3	3	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

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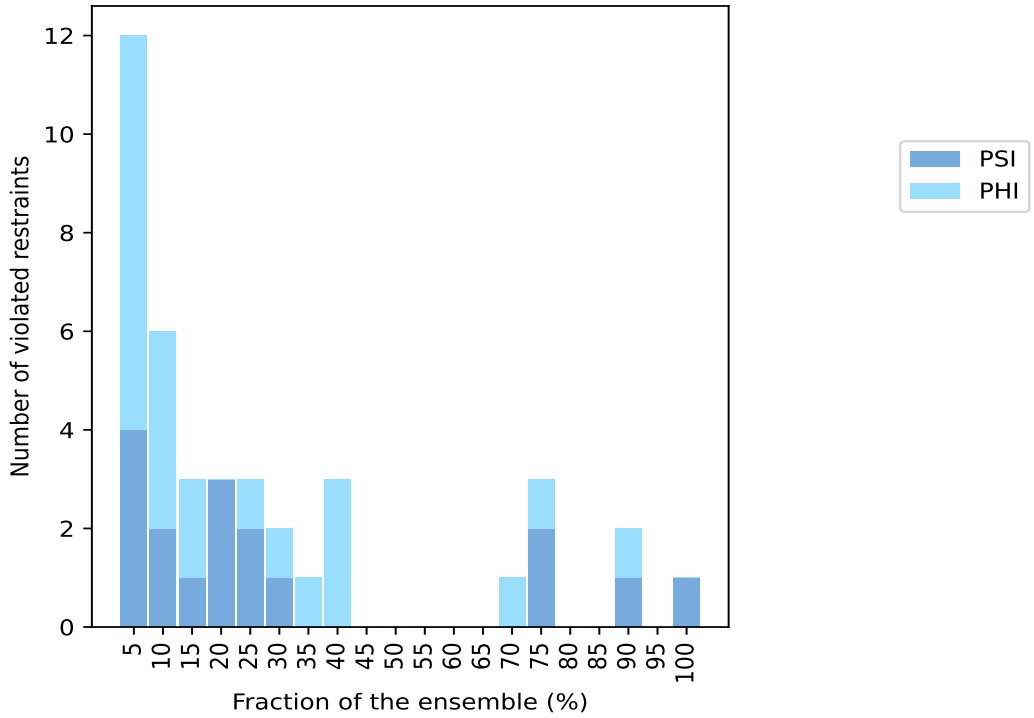
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	1	1	14	70.0
2	1	3	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
1	1	2	18	90.0
0	0	0	19	95.0
1	0	1	20	100.0

[1] Number of models with violations

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

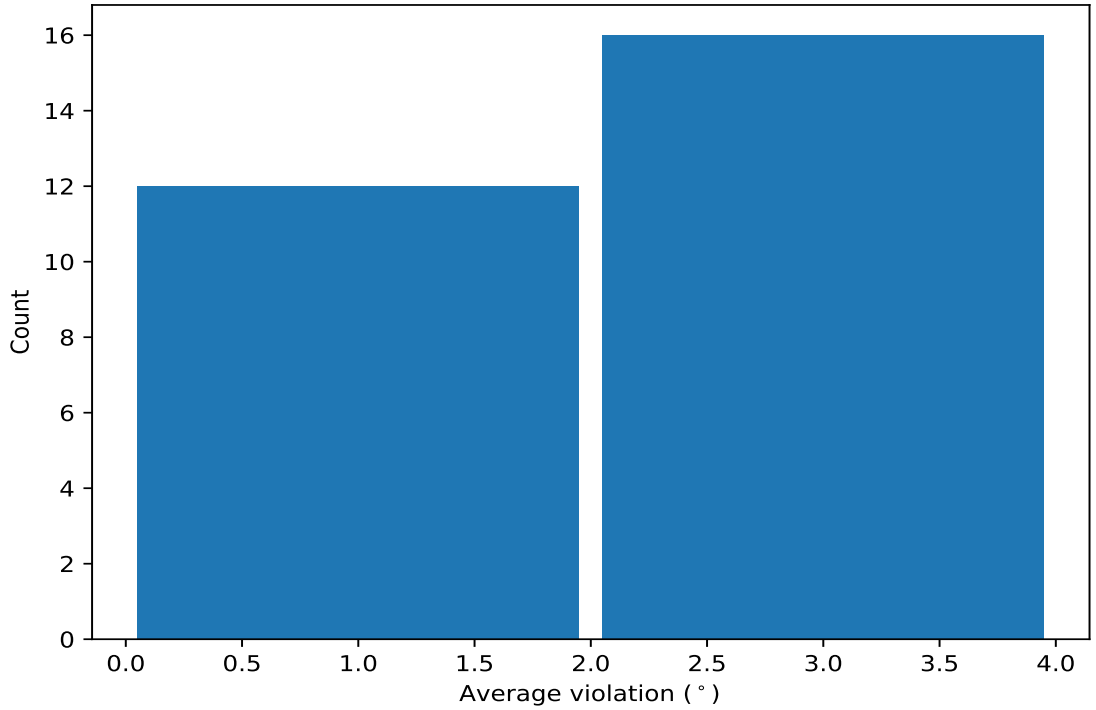


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

The following table provides the mean and the standard deviation of the 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.

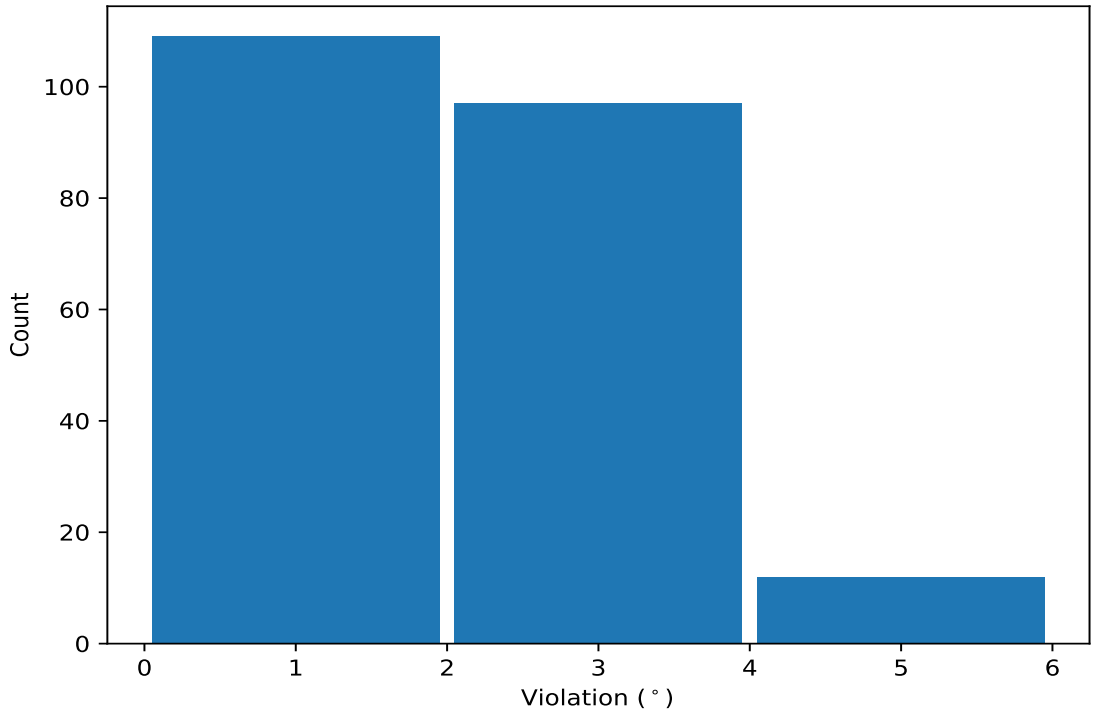
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,32)	1:254:A:TYR:N	1:254:A:TYR:CA	1:254:A:TYR:C	1:255:A:GLY:N	20	2.51	0.71	2.49
(1,61)	1:271:A:CYS:C	1:272:A:SER:N	1:272:A:SER:CA	1:272:A:SER:C	18	3.08	1.13	2.73
(1,18)	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	1:238:A:SER:N	18	1.8	0.7	1.54
(1,92)	1:291:A:ALA:N	1:291:A:ALA:CA	1:291:A:ALA:C	1:292:A:MET:N	15	2.44	0.87	2.82
(1,19)	1:237:A:ILE:C	1:238:A:SER:N	1:238:A:SER:CA	1:238:A:SER:C	15	2.21	0.74	2.02
(1,74)	1:281:A:LYS:N	1:281:A:LYS:CA	1:281:A:LYS:C	1:282:A:HIS:N	15	2.19	0.54	2.15
(1,17)	1:236:A:ALA:C	1:237:A:ILE:N	1:237:A:ILE:CA	1:237:A:ILE:C	14	2.14	0.49	2.14
(1,45)	1:261:A:GLY:C	1:262:A:SER:N	1:262:A:SER:CA	1:262:A:SER:C	8	2.01	0.81	1.95
(1,67)	1:276:A:GLY:C	1:277:A:CYS:N	1:277:A:CYS:CA	1:277:A:CYS:C	8	1.95	0.5	2.03
(1,91)	1:290:A:PRO:C	1:291:A:ALA:N	1:291:A:ALA:CA	1:291:A:ALA:C	8	1.49	0.27	1.5

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,36)	1:257:A:LYS:N	1:257:A:LYS:CA	1:257:A:LYS:C	1:258:A:PRO:N	11	4.74
(1,61)	1:271:A:CYS:C	1:272:A:SER:N	1:272:A:SER:CA	1:272:A:SER:C	15	4.68
(1,32)	1:254:A:TYR:N	1:254:A:TYR:CA	1:254:A:TYR:C	1:255:A:GLY:N	11	4.48
(1,61)	1:271:A:CYS:C	1:272:A:SER:N	1:272:A:SER:CA	1:272:A:SER:C	10	4.44
(1,61)	1:271:A:CYS:C	1:272:A:SER:N	1:272:A:SER:CA	1:272:A:SER:C	11	4.43
(1,61)	1:271:A:CYS:C	1:272:A:SER:N	1:272:A:SER:CA	1:272:A:SER:C	7	4.36
(1,36)	1:257:A:LYS:N	1:257:A:LYS:CA	1:257:A:LYS:C	1:258:A:PRO:N	3	4.34
(1,61)	1:271:A:CYS:C	1:272:A:SER:N	1:272:A:SER:CA	1:272:A:SER:C	16	4.3
(1,61)	1:271:A:CYS:C	1:272:A:SER:N	1:272:A:SER:CA	1:272:A:SER:C	14	4.18
(1,36)	1:257:A:LYS:N	1:257:A:LYS:CA	1:257:A:LYS:C	1:258:A:PRO:N	20	4.13