



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 15, 2026 – 11:36 AM UTC

PDB ID : 2MWG / pdb_00002mwg
BMRB ID : 17643
Title : Full-Length Solution Structure Of YtvA, a LOV-Photoreceptor Protein and Regulator of Bacterial Stress Response
Authors : Jurk, M.; Bardiaux, B.; Schmieder, P.
Deposited on : 2014-11-07

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 : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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 23%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:1-A:261, B:1-B:261 (522)	0.27	1

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. No single-model clusters were found.

Cluster number	Models
1	1, 4, 5, 6, 7, 9
2	8, 10
3	2, 3

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8372 atoms, of which 4218 are hydrogens and 0 are deuteriums.

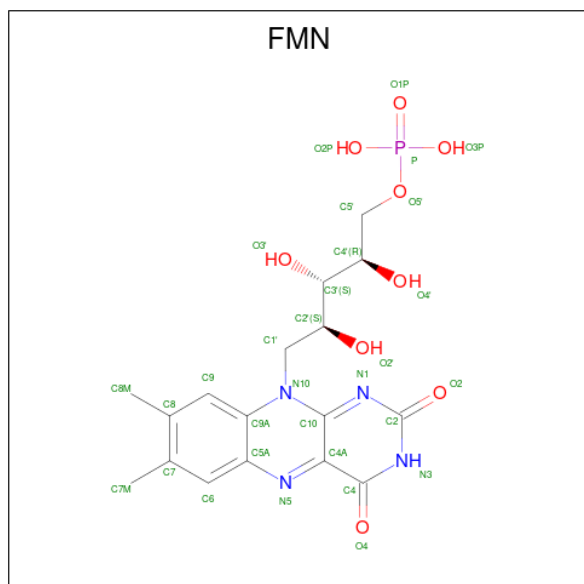
- Molecule 1 is a protein called Blue-light photoreceptor.

Mol	Chain	Residues	Atoms						Trace
1	A	261	Total	C	H	N	O	S	0
			4136	1302	2090	333	403	8	
1	B	261	Total	C	H	N	O	S	0
			4136	1302	2090	333	403	8	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP O34627
B	1	GLY	-	expression tag	UNP O34627

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



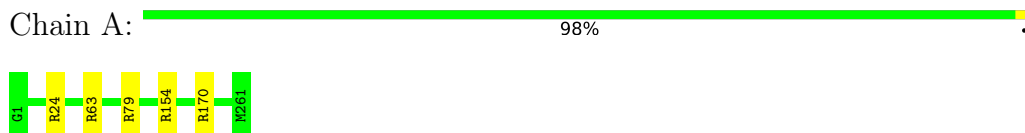
Mol	Chain	Residues	Atoms					
2	A	1	Total	C	H	N	O	P
			50	17	19	4	9	1
2	B	1	Total	C	H	N	O	P
			50	17	19	4	9	1

4 Residue-property plots [i](#)

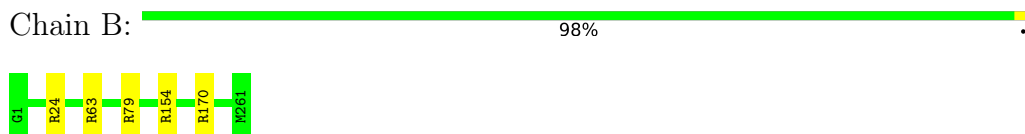
4.1 Average score per residue in the NMR ensemble

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: Blue-light photoreceptor



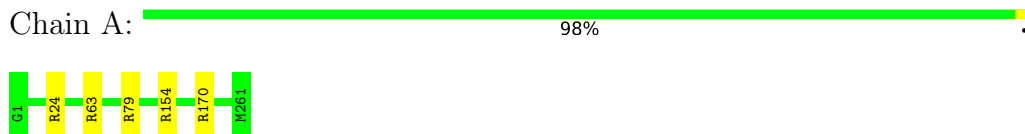
- Molecule 1: Blue-light photoreceptor



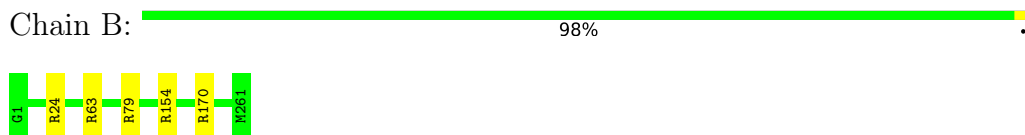
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Blue-light photoreceptor



- Molecule 1: Blue-light photoreceptor



5 Refinement protocol and experimental data overview

The models were refined using the following method: *monte-carlo simulated annealing using torsion angle dynamics, simulated annealing..*

Of the 100 calculated structures, 10 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
CS-ROSETTA	structure solution	v3.2
X-PLOR NIH	structure solution	v2.30
X-PLOR NIH	refinement	v2.30
X-PLOR NIH	geometry optimization	v2.30

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	1643
Number of shifts mapped to atoms	1643
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	23%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

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6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

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 23% for the well-defined parts and 23% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1643
Number of shifts mapped to atoms	1643
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	255	0.22 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	239	0.90 ± 0.09	Should be checked
$^{13}\text{C}'$	255	-0.17 ± 0.11	None needed (< 0.5 ppm)
^{15}N	242	-0.45 ± 0.12	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 23%, i.e. 1632 atoms were assigned a chemical shift out of a possible 7174. 0 out of 94 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	994/2596 (38%)	242/1052 (23%)	510/1044 (49%)	242/500 (48%)
Sidechain	636/4200 (15%)	306/2736 (11%)	330/1334 (25%)	0/130 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	2/378 (1%)	1/182 (1%)	0/182 (0%)	1/14 (7%)
Overall	1632/7174 (23%)	549/3970 (14%)	840/2560 (33%)	243/644 (38%)

7.1.4 Statistically unusual chemical shifts [i](#)

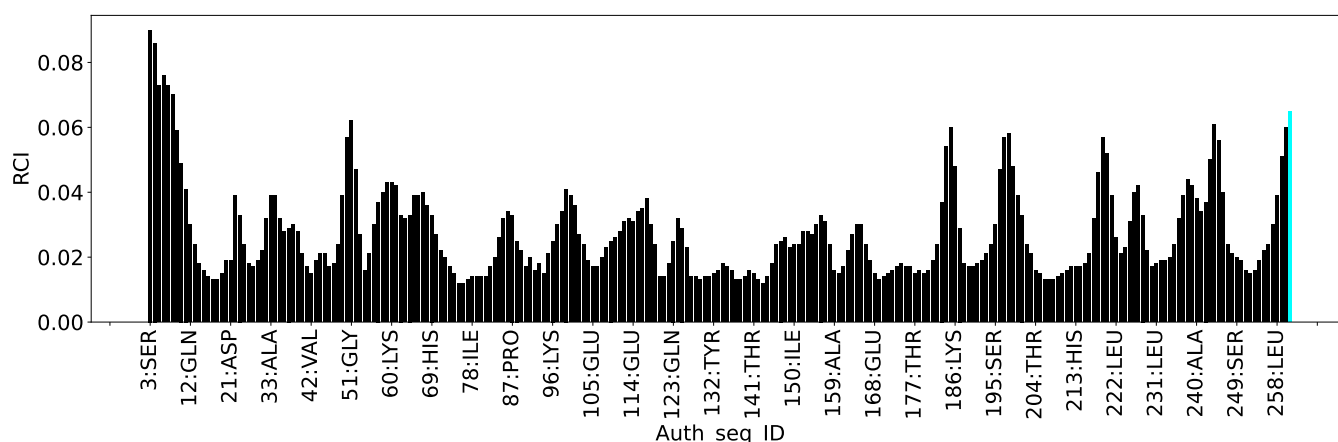
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	204	THR	HG1	5.87	0.08 – 2.19	22.4
1	A	247	THR	HG1	5.59	0.08 – 2.19	21.1
1	A	225	THR	HG1	5.38	0.08 – 2.19	20.1
1	A	179	THR	HG1	5.07	0.08 – 2.19	18.6
1	A	70	THR	HG1	4.93	0.08 – 2.19	18.0
1	A	30	THR	HG1	4.89	0.08 – 2.19	17.8
1	A	148	THR	HG1	4.74	0.08 – 2.19	17.1
1	A	220	THR	HG1	4.36	0.08 – 2.19	15.3

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	1192
Intra-residue ($ i-j =0$)	58
Sequential ($ i-j =1$)	452
Medium range ($ i-j >1$ and $ i-j <5$)	380
Long range ($ i-j \geq 5$)	294
Inter-chain	0
Hydrogen bond restraints	8
Disulfide bond restraints	0
Total dihedral-angle restraints	814
Number of unmapped restraints	0
Number of restraints per residue	3.8
Number of long range restraints per residue ¹	0.6

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)	56.5	0.2
0.2-0.5 (Medium)	24.6	0.5
>0.5 (Large)	2.4	0.88

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)	46.2	9.98
10.0-20.0 (Medium)	7.1	19.89
>20.0 (Large)	1.5	22.97

9 Distance violation analysis ⓘ

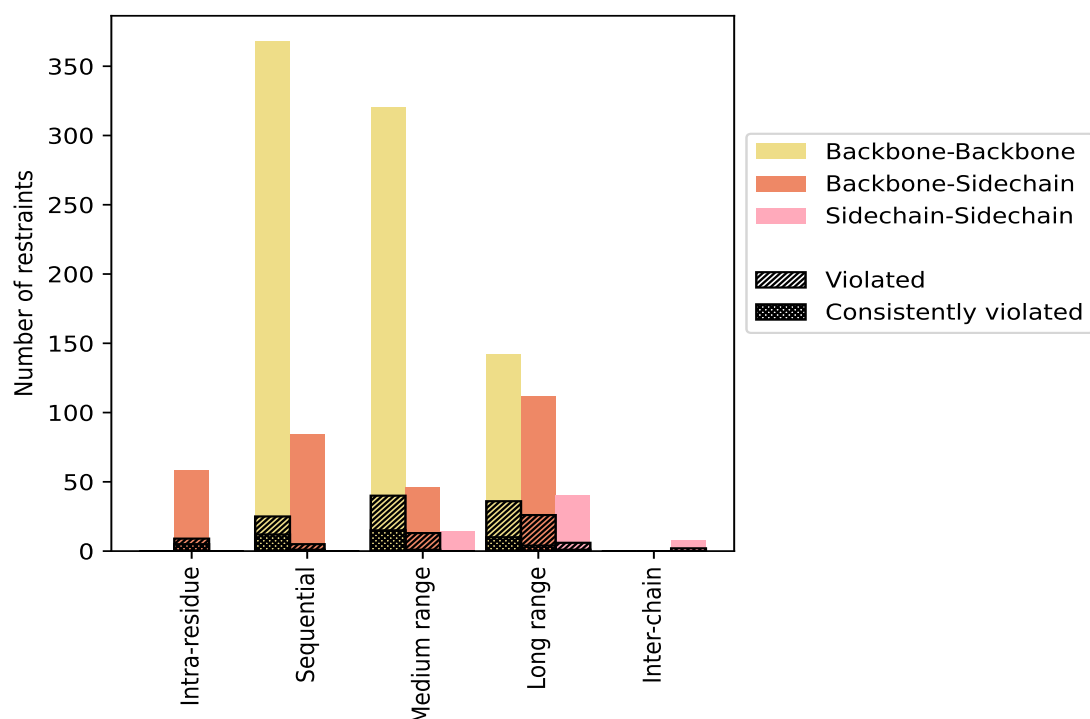
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	58	4.9	9	15.5	0.8	5	8.6	0.4
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	58	4.9	9	15.5	0.8	5	8.6	0.4
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	452	37.9	30	6.6	2.5	13	2.9	1.1
Backbone-Backbone	368	30.9	25	6.8	2.1	12	3.3	1.0
Backbone-Sidechain	84	7.0	5	6.0	0.4	1	1.2	0.1
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	380	31.9	53	13.9	4.4	16	4.2	1.3
Backbone-Backbone	320	26.8	40	12.5	3.4	15	4.7	1.3
Backbone-Sidechain	46	3.9	13	28.3	1.1	1	2.2	0.1
Sidechain-Sidechain	14	1.2	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	294	24.7	68	23.1	5.7	15	5.1	1.3
Backbone-Backbone	142	11.9	36	25.4	3.0	10	7.0	0.8
Backbone-Sidechain	112	9.4	26	23.2	2.2	4	3.6	0.3
Sidechain-Sidechain	40	3.4	6	15.0	0.5	1	2.5	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	8	0.7	2	25.0	0.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1192	100.0	162	13.6	13.6	49	4.1	4.1
Backbone-Backbone	830	69.6	101	12.2	8.5	37	4.5	3.1
Backbone-Sidechain	300	25.2	53	17.7	4.4	11	3.7	0.9
Sidechain-Sidechain	62	5.2	8	12.9	0.7	1	1.6	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 [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

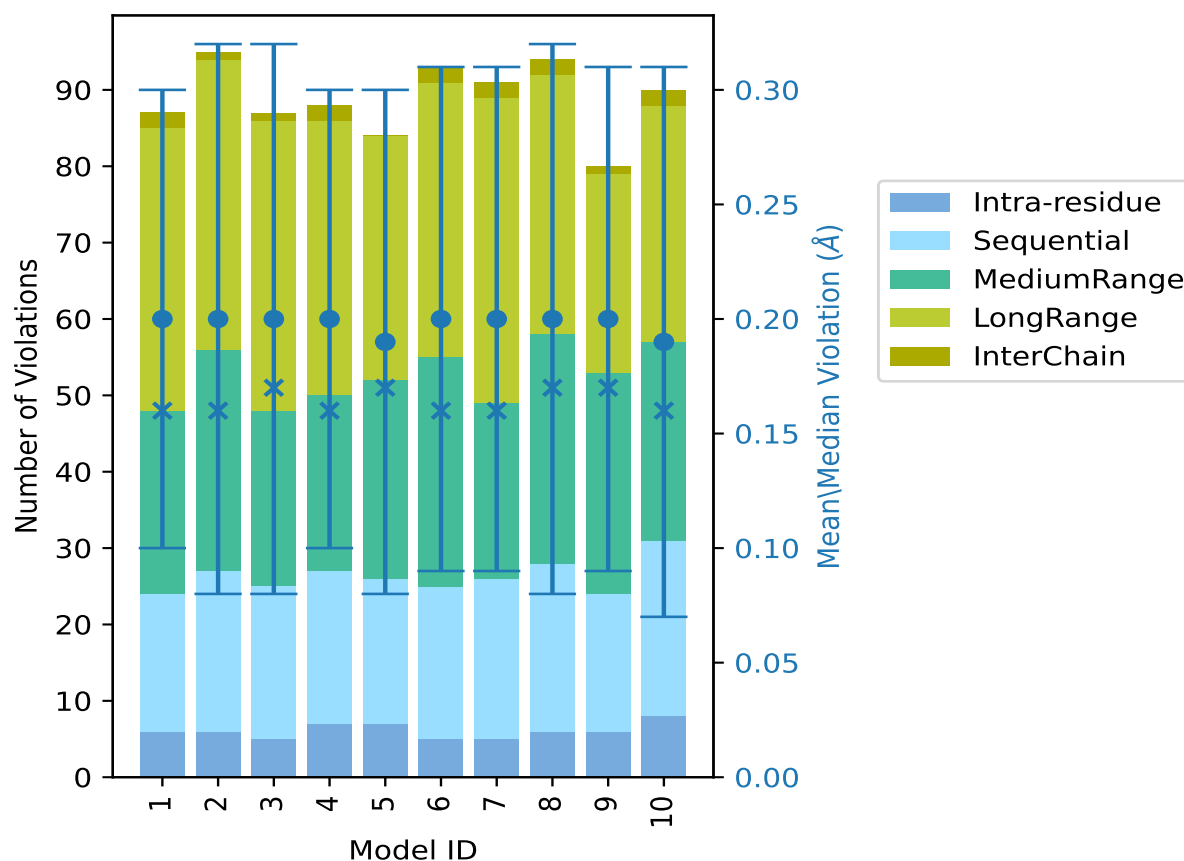
9.2 Distance violation statistics for each model [i](#)

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	6	18	24	37	2	87	0.2	0.67	0.1	0.16
2	6	21	29	38	1	95	0.2	0.88	0.12	0.16
3	5	20	23	38	1	87	0.2	0.8	0.12	0.17
4	7	20	23	36	2	88	0.2	0.6	0.1	0.16
5	7	19	26	32	0	84	0.19	0.74	0.11	0.17
6	5	20	30	36	2	93	0.2	0.79	0.11	0.16
7	5	21	23	40	2	91	0.2	0.71	0.11	0.16
8	6	22	30	34	2	94	0.2	0.84	0.12	0.17
9	6	18	29	26	1	80	0.2	0.66	0.11	0.17
10	8	23	26	31	2	90	0.19	0.82	0.12	0.16

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 [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, 1024(IR:49, SQ:422, MR:327, LR:226, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	1	14	15	0	30	1	10.0
1	6	9	7	0	23	2	20.0
3	2	4	8	0	17	3	30.0

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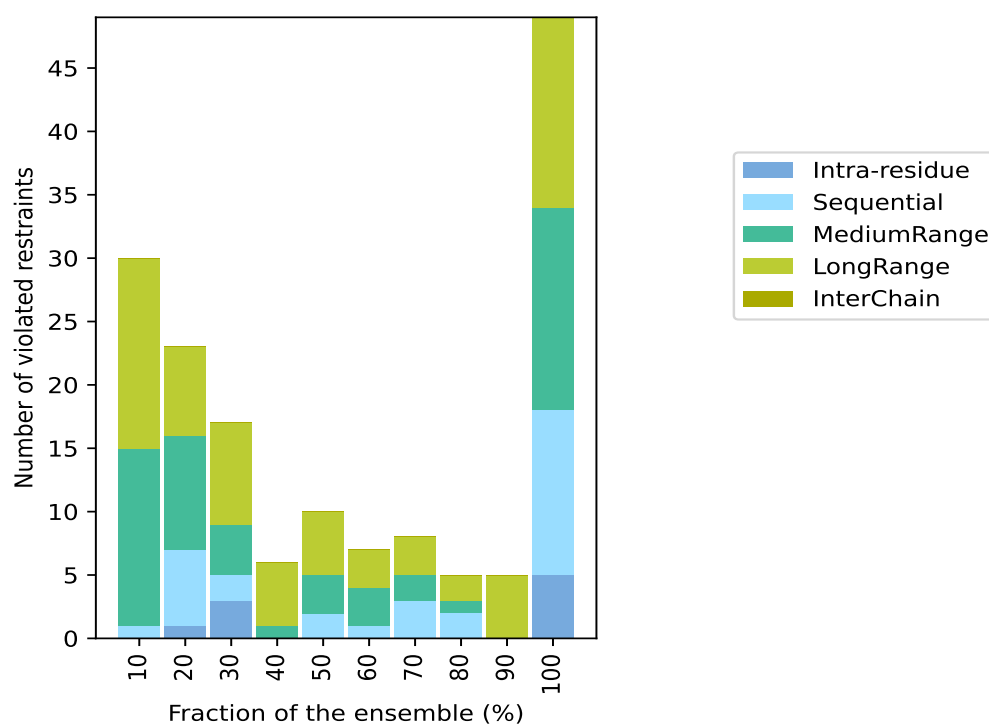
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	1	5	0	6	4	40.0
0	2	3	5	0	10	5	50.0
0	1	3	3	0	7	6	60.0
0	3	2	3	0	8	7	70.0
0	2	1	2	0	5	8	80.0
0	0	0	5	0	5	9	90.0
5	13	16	15	0	49	10	100.0

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](#)

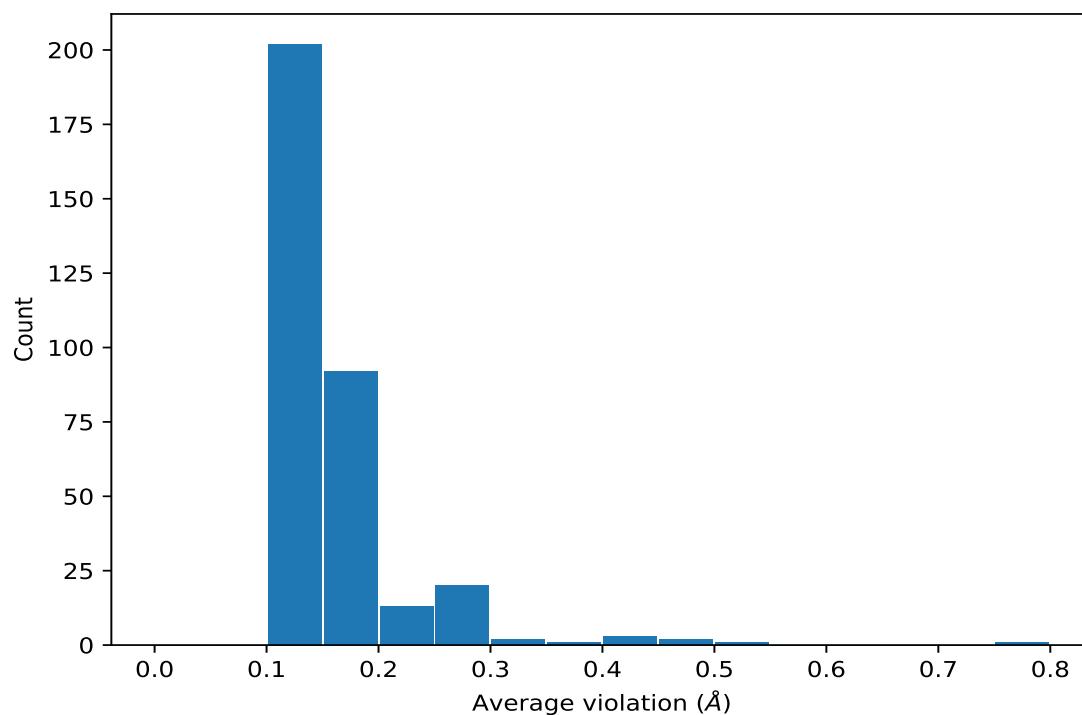


9.4 Most violated distance restraints in the ensemble [i](#)

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.

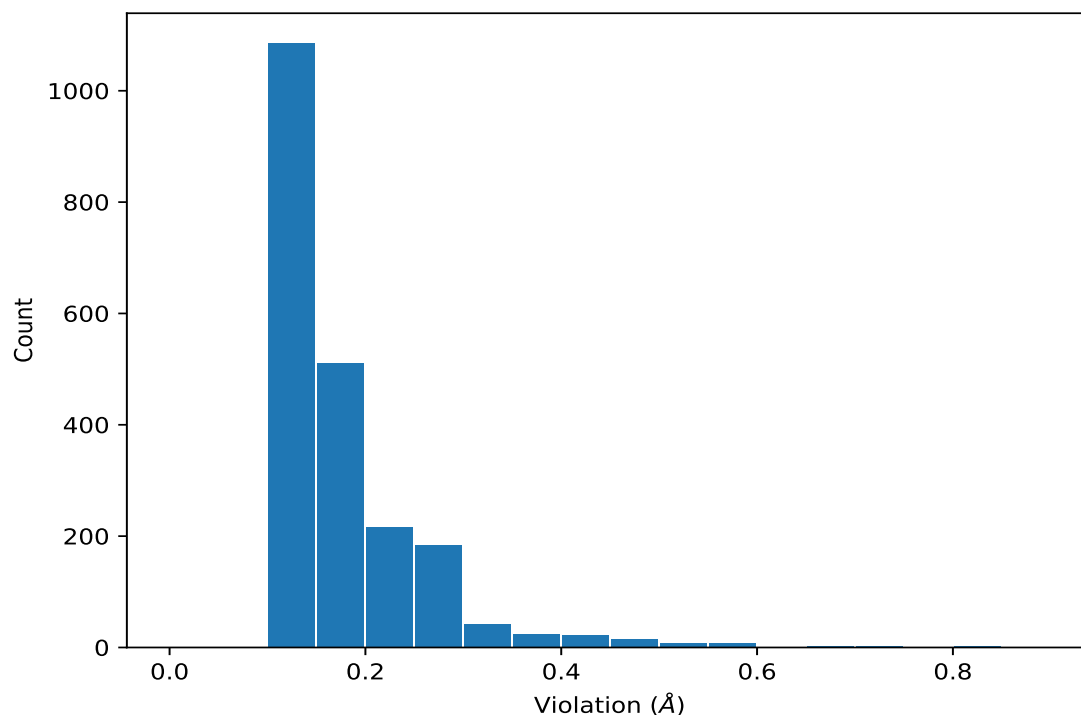
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	10	0.75	0.09	0.76
(2,1144)	1:239:B:ASP:H	1:241:B:ASN:H	10	0.53	0.02	0.54
(2,630)	1:30:B:THR:H	1:119:B:PHE:H	10	0.45	0.04	0.44
(2,821)	1:96:B:LYS:H	1:99:B:GLY:H	10	0.45	0.03	0.44
(2,817)	1:94:B:ASN:H	1:102:B:PHE:H	10	0.42	0.03	0.44
(2,976)	1:166:B:LEU:H	1:201:B:ASN:H	10	0.42	0.09	0.4
(2,935)	1:151:B:VAL:H	1:159:B:ALA:H	10	0.42	0.06	0.4
(2,1113)	1:224:B:ILE:H	1:248:B:TYR:H	10	0.37	0.04	0.37
(2,1142)	1:238:B:LEU:H	1:240:B:ALA:H	10	0.31	0.02	0.3
(2,828)	1:98:B:ASP:H	1:100:B:THR:H	10	0.31	0.02	0.3

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)
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	2	0.88
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	8	0.84
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	10	0.82
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	3	0.8
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	6	0.79
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	5	0.74
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	7	0.71
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	1	0.67
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	9	0.66
(2,722)	1:67:B:GLY:H	1:95:B:TYR:H	4	0.6

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

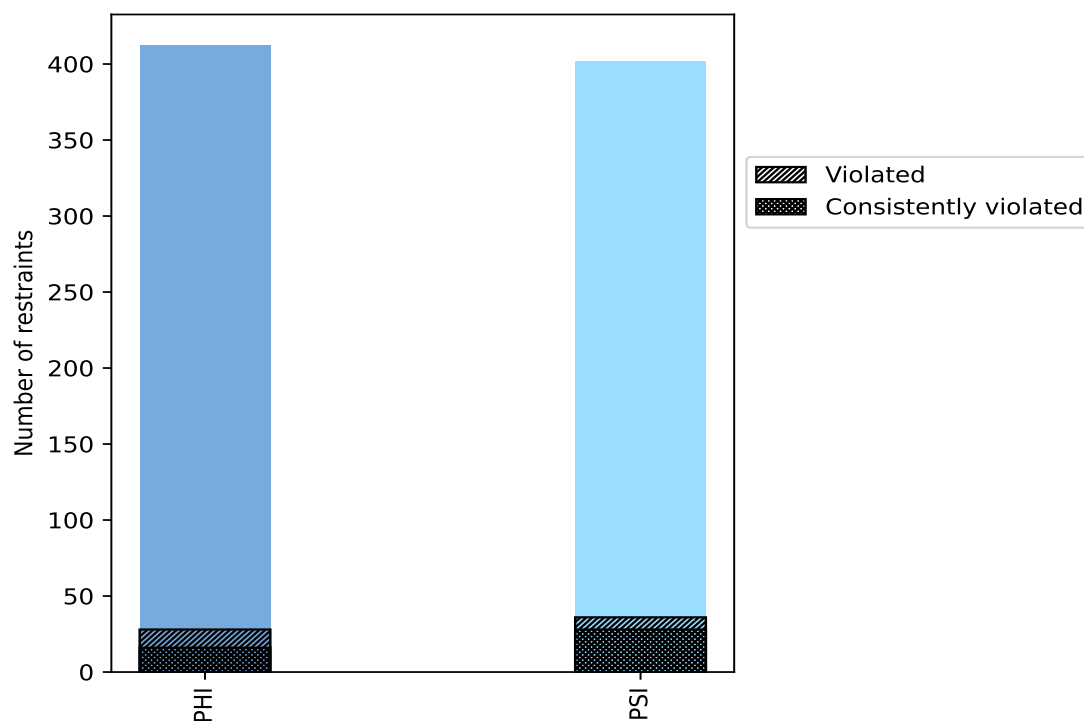
10.1 Summary of dihedral-angle violations [i](#)

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
PHI	412	50.6	28	6.8	3.4	16	3.9	2.0
PSI	402	49.4	36	9.0	4.4	28	7.0	3.4
Total	814	100.0	64	7.9	7.9	44	5.4	5.4

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](#)



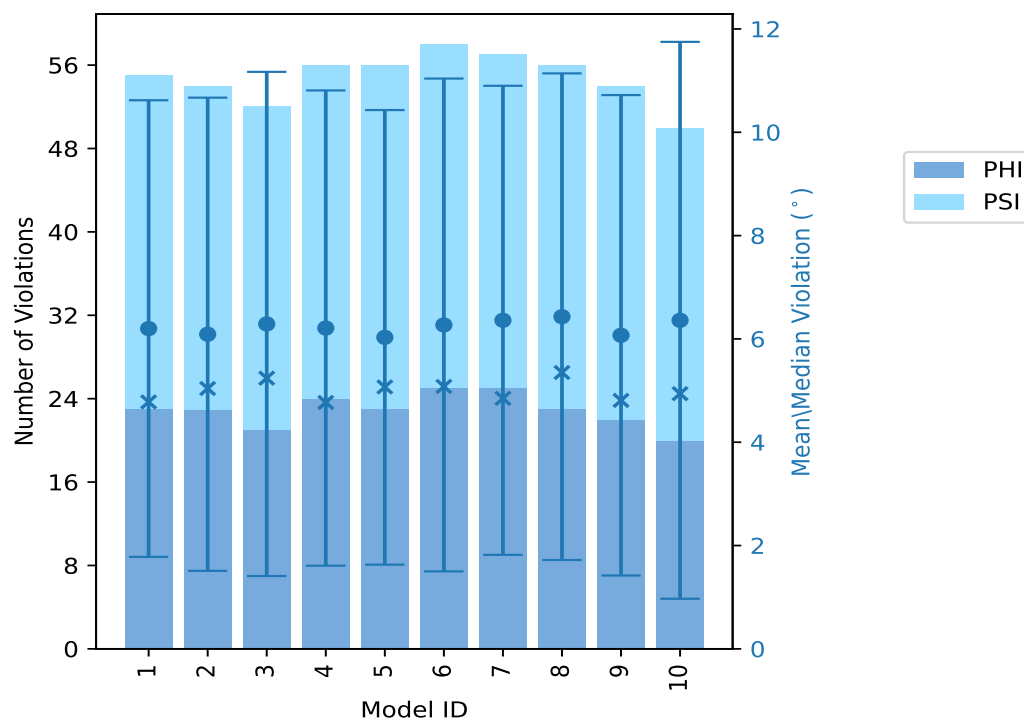
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PHI	PSI	Total				
1	23	32	55	6.2	19.8	4.42	4.78
2	23	31	54	6.09	21.26	4.58	5.04
3	21	31	52	6.29	20.81	4.88	5.24
4	24	32	56	6.21	20.14	4.6	4.77
5	23	33	56	6.03	20.41	4.4	5.07
6	25	33	58	6.27	22.14	4.77	5.08
7	25	32	57	6.36	19.82	4.54	4.85
8	23	33	56	6.43	21.09	4.71	5.35
9	22	32	54	6.07	19.56	4.65	4.81
10	20	30	50	6.36	22.97	5.39	4.94

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

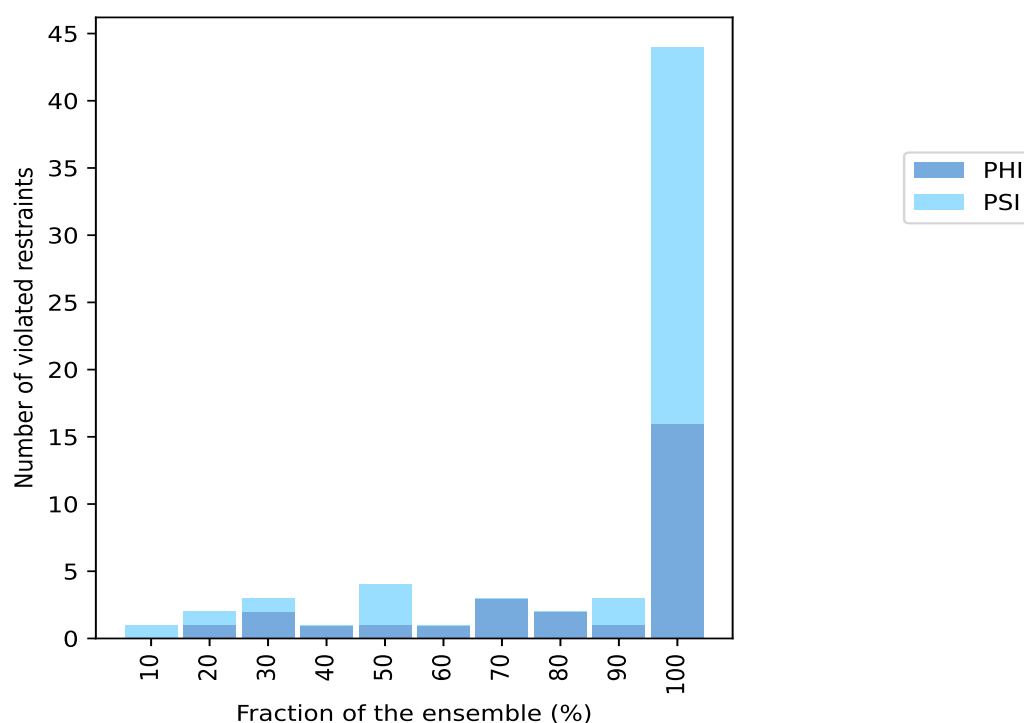
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	1	1	1	10.0
1	1	2	2	20.0
2	1	3	3	30.0
1	0	1	4	40.0
1	3	4	5	50.0
1	0	1	6	60.0
3	0	3	7	70.0
2	0	2	8	80.0
1	2	3	9	90.0
16	28	44	10	100.0

¹ Number of models with violations

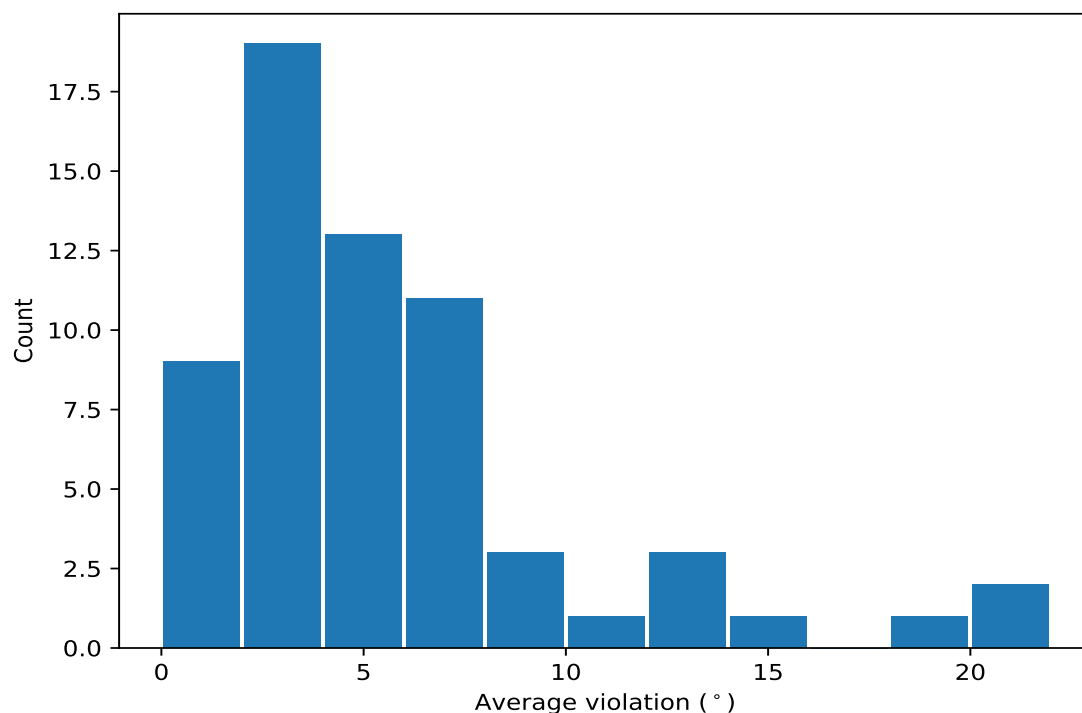
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

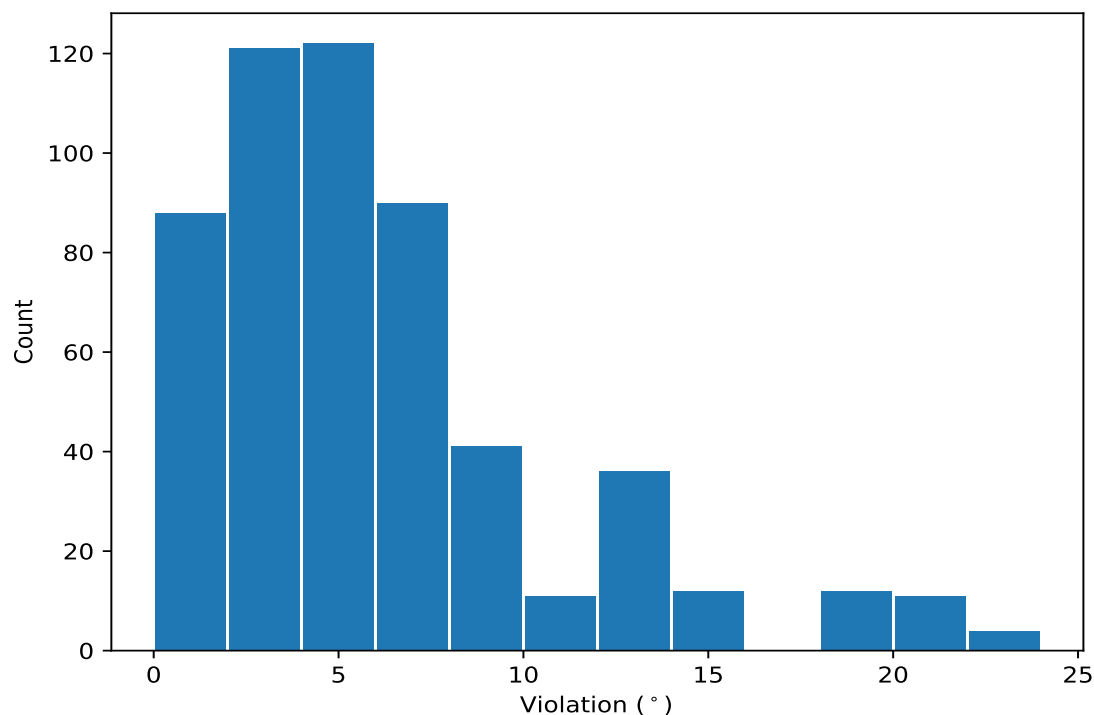
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,226)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:TYR:N	10	20.51	1.22	20.27
(1,633)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:TYR:N	10	20.25	1.14	19.96
(1,196)	1:245:A:LEU:C	1:246:A:LYS:N	1:246:A:LYS:CA	1:246:A:LYS:C	10	18.16	3.88	18.86
(1,579)	1:217:B:LEU:C	1:218:B:THR:N	1:218:B:THR:CA	1:218:B:THR:C	10	14.74	0.7	14.99
(1,172)	1:217:A:LEU:C	1:218:A:THR:N	1:218:A:THR:CA	1:218:A:THR:C	10	13.57	0.48	13.66
(1,336)	1:177:A:THR:N	1:177:A:THR:CA	1:177:A:THR:C	1:178:A:LEU:N	10	13.22	0.36	13.26
(1,743)	1:177:B:THR:N	1:177:B:THR:CA	1:177:B:THR:C	1:178:B:LEU:N	10	13.15	0.47	13.25
(1,519)	1:149:B:PRO:C	1:150:B:ILE:N	1:150:B:ILE:CA	1:150:B:ILE:C	10	11.75	1.0	12.2
(1,612)	1:256:B:LYS:C	1:257:B:VAL:N	1:257:B:VAL:CA	1:257:B:VAL:C	10	8.42	0.39	8.42
(1,680)	1:101:B:MET:N	1:101:B:MET:CA	1:101:B:MET:C	1:102:B:PHE:N	10	8.27	1.05	8.35

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 (°)
(1,226)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:TYR:N	10	22.97
(1,196)	1:245:A:LEU:C	1:246:A:LYS:N	1:246:A:LYS:CA	1:246:A:LYS:C	10	22.67
(1,633)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:TYR:N	10	22.44
(1,226)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:TYR:N	6	22.14
(1,633)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:TYR:N	6	21.77
(1,196)	1:245:A:LEU:C	1:246:A:LYS:N	1:246:A:LYS:CA	1:246:A:LYS:C	6	21.54
(1,226)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:TYR:N	2	21.26
(1,196)	1:245:A:LEU:C	1:246:A:LYS:N	1:246:A:LYS:CA	1:246:A:LYS:C	8	21.09
(1,633)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:TYR:N	2	21.06
(1,196)	1:245:A:LEU:C	1:246:A:LYS:N	1:246:A:LYS:CA	1:246:A:LYS:C	3	20.81