



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 15, 2026 – 11:36 AM UTC

PDB ID : 6V4T / pdb_00006v4t
BMRB ID : 30503
Title : MPER-TMD of HIV-1 Env bound with the entry inhibitor S2C3
Authors : Xiao, T.; Frey, G.; Fu, Q.; Lavine, C.L.; Scott, D.A.; Seaman, M.S.; Chou, J.J.; Chen, B.
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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 4%.

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 14 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:660-A:710, B:660-B:710, C:660-C:709 (152)	1.83	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 and 2 single-model clusters were found.

Cluster number	Models
1	3, 4, 8, 9, 11
2	1, 6, 7, 12
3	2, 13, 14
Single-model clusters	5; 10

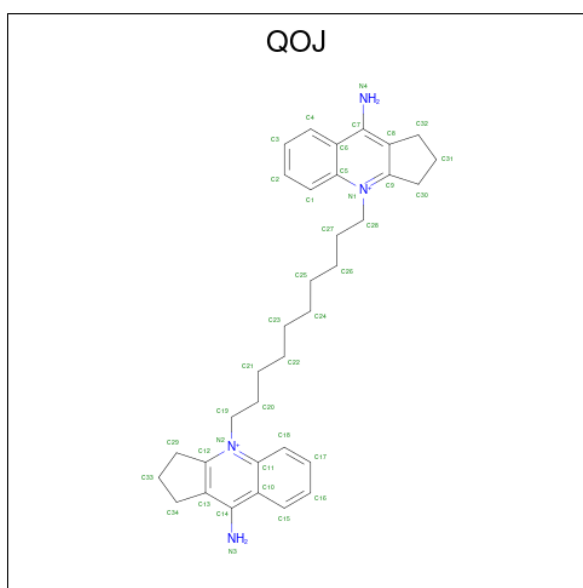
3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2958 atoms, of which 1521 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					Trace
1	A	51	Total	C	H	N	O	0
			904	301	463	73	67	
1	B	51	Total	C	H	N	O	0
			904	301	463	73	67	
1	C	51	Total	C	H	N	O	0
			904	301	463	73	67	

- Molecule 2 is 4,4'-(decane-1,10-diyl)bis(9-amino-2,3-dihydro-1H-cyclopenta[b]quinolin-4-ium m) (CCD ID: QOJ) (formula: C₃₄H₄₄N₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			
2	A	1	Total	C	H	N
			82	34	44	4
2	B	1	Total	C	H	N
			82	34	44	4
2	C	1	Total	C	H	N
			82	34	44	4

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: Envelope glycoprotein gp160

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain C:  98%



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: Envelope glycoprotein gp160

Chain A:  100%

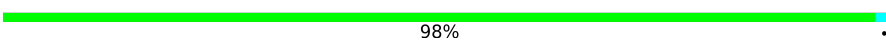
There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 1: Envelope glycoprotein gp160

Chain C:  98%



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 14 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	refinement	
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	96
Number of shifts mapped to atoms	96
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	4%

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](#)

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6.3.2 Protein sidechains [i](#)

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6.3.3 RNA [i](#)

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

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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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 4% for the well-defined parts and 4% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *BMRB.txt*

7.1.1 Bookkeeping [i](#)

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

Total number of shifts	96
Number of shifts mapped to atoms	96
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	48	1.55 ± 0.88	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 4%, i.e. 96 atoms were assigned a chemical shift out of a possible 2409. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	96/766 (13%)	48/310 (15%)	0/304 (0%)	48/152 (32%)
Sidechain	0/1346 (0%)	0/894 (0%)	0/402 (0%)	0/50 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/297 (0%)	0/147 (0%)	0/135 (0%)	0/15 (0%)
Overall	96/2409 (4%)	48/1351 (4%)	0/841 (0%)	48/217 (22%)

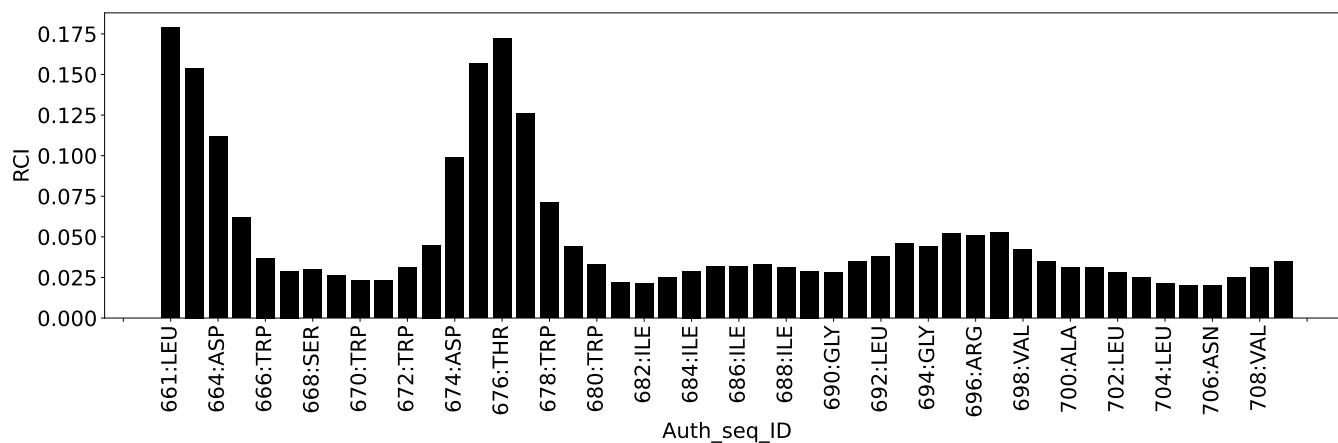
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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	669
Intra-residue ($ i-j =0$)	83
Sequential ($ i-j =1$)	288
Medium range ($ i-j >1$ and $ i-j <5$)	267
Long range ($ i-j \geq 5$)	25
Inter-chain	6
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	84
Number of unmapped restraints	0
Number of restraints per residue	4.8
Number of long range restraints per residue ¹	0.2

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)	39.2	0.2
0.2-0.5 (Medium)	29.3	0.5
>0.5 (Large)	31.3	27.53

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)	7.9	4.01
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

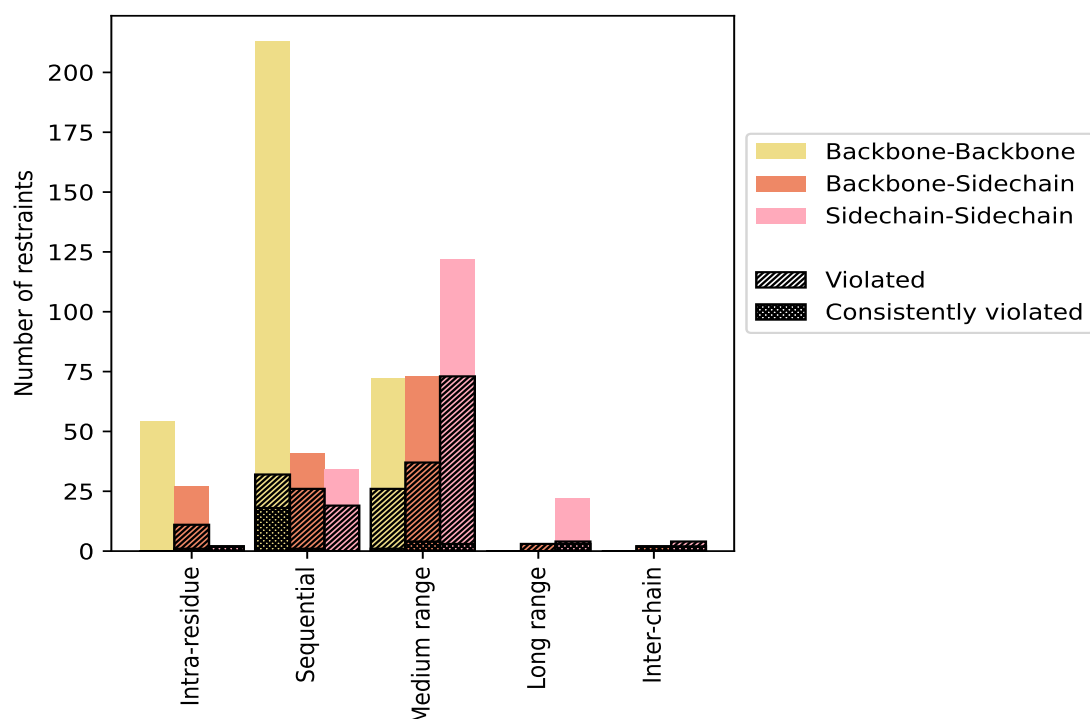
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	83	12.4	13	15.7	1.9	3	3.6	0.4
Backbone-Backbone	54	8.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	27	4.0	11	40.7	1.6	1	3.7	0.1
Sidechain-Sidechain	2	0.3	2	100.0	0.3	2	100.0	0.3
Sequential ($i-j =1$)	288	43.0	77	26.7	11.5	19	6.6	2.8
Backbone-Backbone	213	31.8	32	15.0	4.8	18	8.5	2.7
Backbone-Sidechain	41	6.1	26	63.4	3.9	1	2.4	0.1
Sidechain-Sidechain	34	5.1	19	55.9	2.8	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	267	39.9	136	50.9	20.3	8	3.0	1.2
Backbone-Backbone	72	10.8	26	36.1	3.9	1	1.4	0.1
Backbone-Sidechain	73	10.9	37	50.7	5.5	4	5.5	0.6
Sidechain-Sidechain	122	18.2	73	59.8	10.9	3	2.5	0.4
Long range ($i-j \geq 5$)	25	3.7	7	28.0	1.0	3	12.0	0.4
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	3	0.4	3	100.0	0.4	0	0.0	0.0
Sidechain-Sidechain	22	3.3	4	18.2	0.6	3	13.6	0.4
Inter-chain	6	0.9	6	100.0	0.9	4	66.7	0.6
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2	0.3	2	100.0	0.3	2	100.0	0.3
Sidechain-Sidechain	4	0.6	4	100.0	0.6	2	50.0	0.3
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	669	100.0	239	35.7	35.7	37	5.5	5.5
Backbone-Backbone	339	50.7	58	17.1	8.7	19	5.6	2.8
Backbone-Sidechain	146	21.8	79	54.1	11.8	8	5.5	1.2
Sidechain-Sidechain	184	27.5	102	55.4	15.2	10	5.4	1.5

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 disulfied 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	4	41	41	4	4	94	1.3	24.54	3.79	0.25
2	9	34	43	4	5	95	1.35	21.48	3.52	0.23
3	4	47	41	4	4	100	1.19	22.03	3.31	0.3
4	8	37	49	4	5	103	1.18	20.42	3.15	0.27
5	6	44	47	4	5	106	1.19	24.63	3.48	0.25
6	10	44	47	4	5	110	1.07	18.2	2.83	0.24
7	7	34	43	4	5	93	1.42	26.6	4.08	0.2
8	10	41	50	4	5	110	1.12	25.21	3.4	0.21
9	4	43	47	4	5	103	1.29	27.01	3.86	0.23
10	4	39	37	4	5	89	1.46	24.66	3.81	0.26

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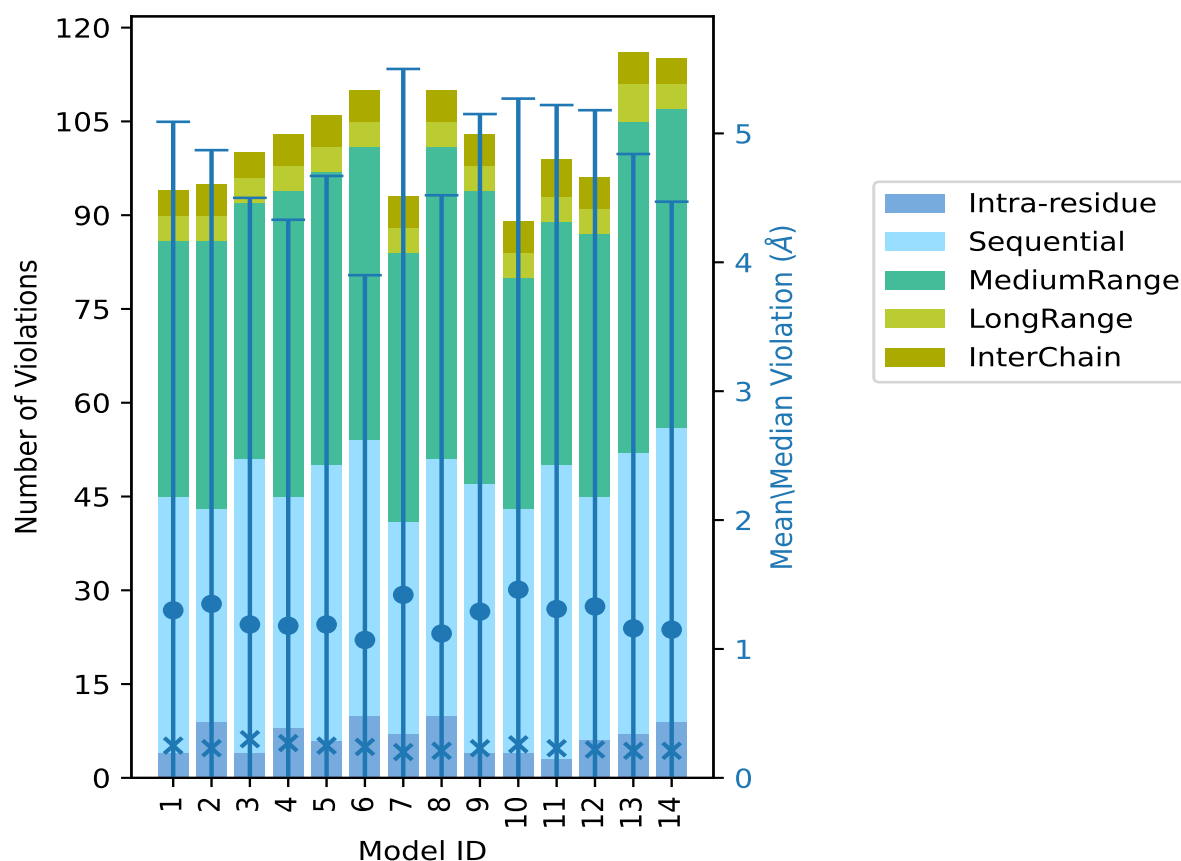
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	3	47	39	4	6	99	1.31	27.53	3.91	0.23
12	6	39	42	4	5	96	1.33	26.04	3.85	0.22
13	7	45	53	6	5	116	1.16	26.91	3.68	0.21
14	9	47	51	4	4	115	1.15	24.73	3.32	0.21

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

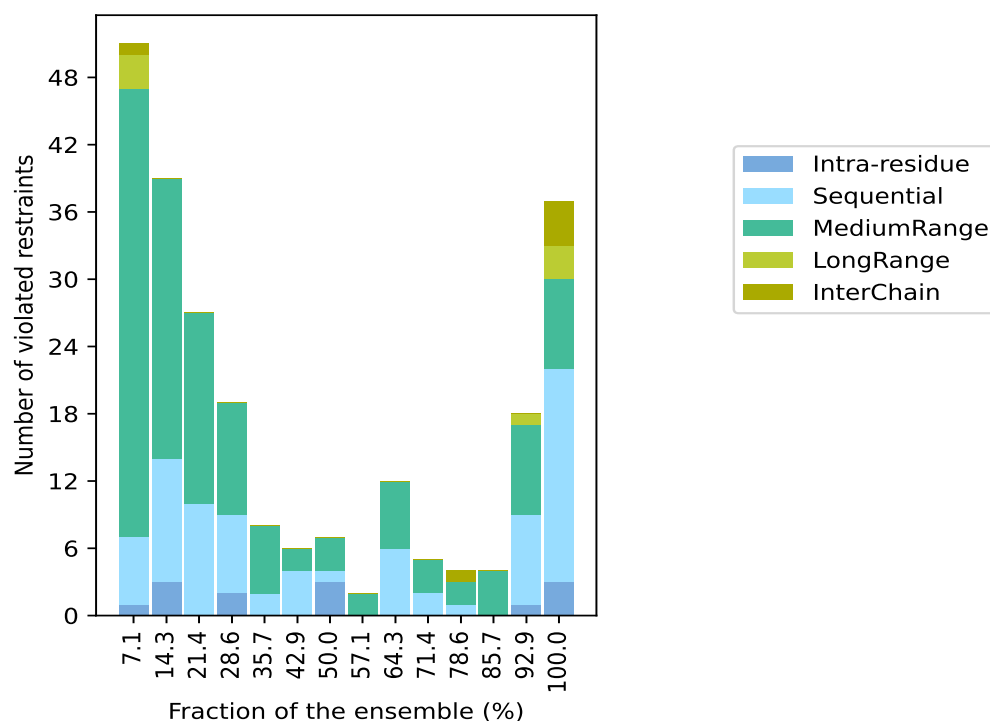
for a given fraction of the ensemble. In total, 430(IR:70, SQ:211, MR:131, LR:18, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	6	40	3	1	51	1	7.1
3	11	25	0	0	39	2	14.3
0	10	17	0	0	27	3	21.4
2	7	10	0	0	19	4	28.6
0	2	6	0	0	8	5	35.7
0	4	2	0	0	6	6	42.9
3	1	3	0	0	7	7	50.0
0	0	2	0	0	2	8	57.1
0	6	6	0	0	12	9	64.3
0	2	3	0	0	5	10	71.4
0	1	2	0	1	4	11	78.6
0	0	4	0	0	4	12	85.7
1	8	8	1	0	18	13	92.9
3	19	8	3	4	37	14	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

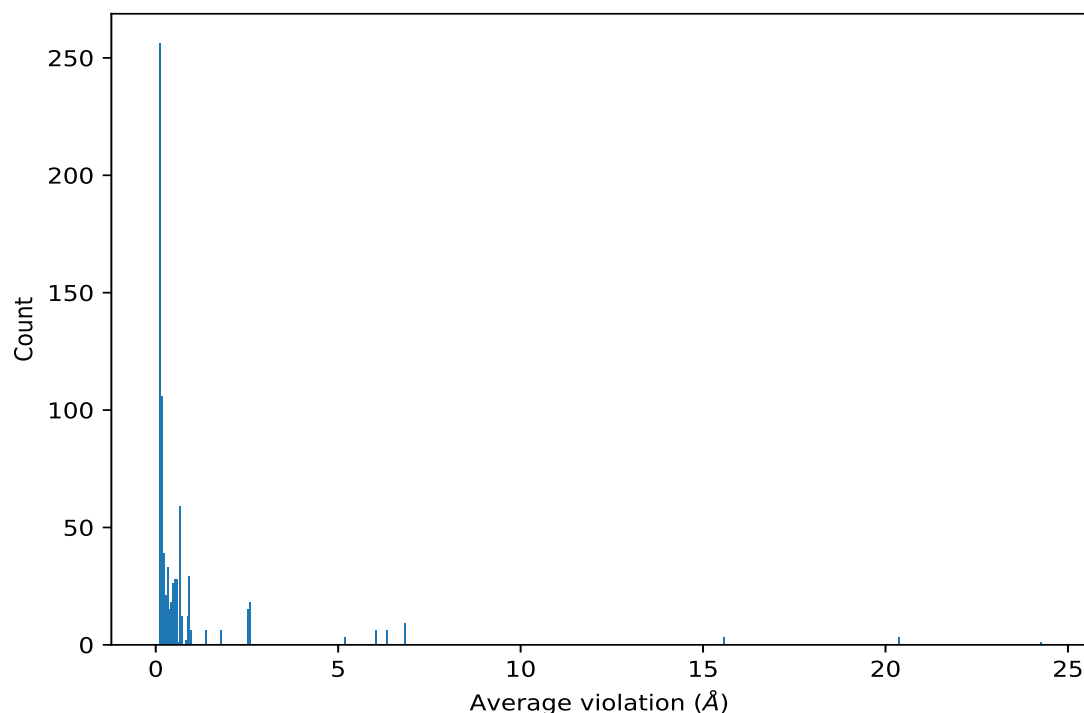
9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ



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

9.4.1 Histogram : Distribution of mean distance violations [i](#)

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



9.4.2 Table: Most violated distance restraints [i](#)

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	14	24.29	2.67	24.7
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	14	20.36	1.69	20.49
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	14	20.36	1.69	20.49
(1,2)	1:672:A:TRP:HE1	2:801:B:QOJ:H151	14	20.36	1.69	20.49
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	14	15.55	1.23	15.22
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	14	15.55	1.23	15.22
(1,4)	1:675:A:ILE:H	2:801:B:QOJ:H181	14	15.55	1.23	15.22
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	6.83	0.47	6.74
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	6.83	0.47	6.74

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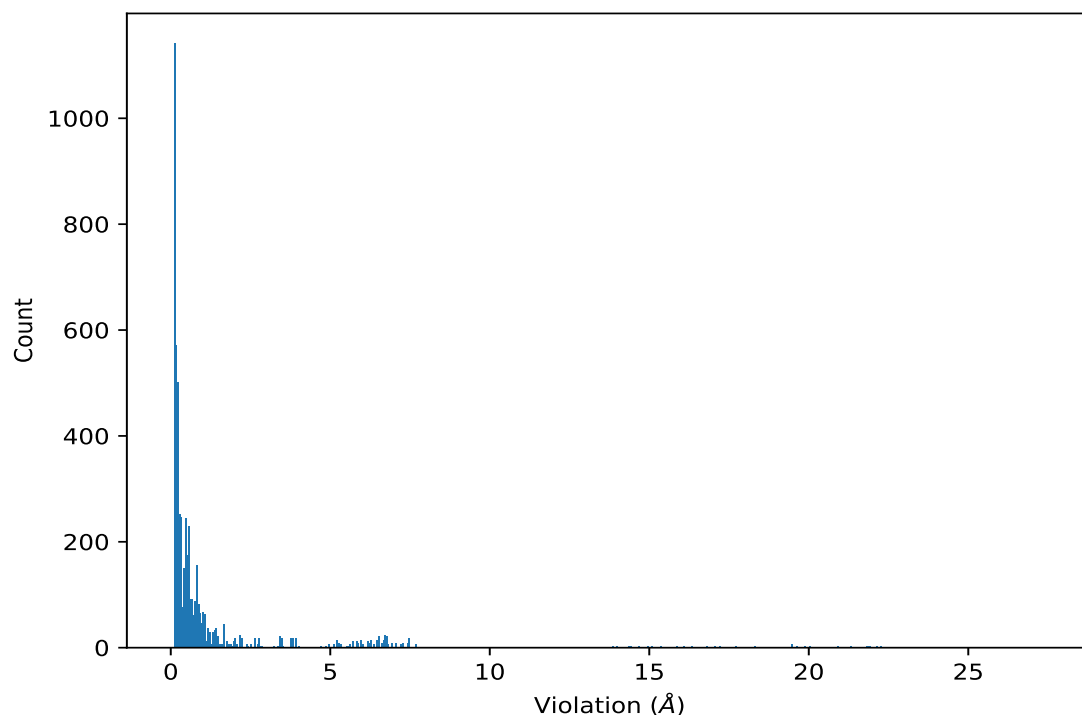
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	6.83	0.47	6.74
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	6.83	0.47	6.74
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	6.83	0.47	6.74
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	6.83	0.47	6.74
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD11	14	6.83	0.47	6.74
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD12	14	6.83	0.47	6.74
(2,8)	1:678:A:TRP:HE1	1:687:A:ILE:HD13	14	6.83	0.47	6.74
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	6.34	0.65	6.31
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	6.34	0.65	6.31
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	6.34	0.65	6.31
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	6.34	0.65	6.31
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB2	14	6.34	0.65	6.31
(2,6)	1:670:A:TRP:HE1	1:660:A:LEU:HB3	14	6.34	0.65	6.31
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	14	6.03	0.56	6.07
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	14	6.03	0.56	6.07
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	14	6.03	0.56	6.07
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	14	6.03	0.56	6.07
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H271	14	6.03	0.56	6.07
(1,5)	1:661:A:LEU:H	2:801:B:QOJ:H272	14	6.03	0.56	6.07
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	5.18	0.91	5.24
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	5.18	0.91	5.24
(2,7)	1:678:A:TRP:HE1	1:683:A:ARG:HE	14	5.18	0.91	5.24
(2,18)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	14	2.54	1.27	2.18
(2,18)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	14	2.54	1.27	2.18
(2,18)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	14	2.54	1.27	2.18
(2,18)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	14	2.54	1.27	2.18
(2,18)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	14	2.54	1.27	2.18
(2,19)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	14	2.54	1.27	2.18
(2,19)	1:693:A:ILE:HD12	1:696:A:ARG:HH21	14	2.54	1.27	2.18
(2,19)	1:693:A:ILE:HD12	1:696:A:ARG:HH11	14	2.54	1.27	2.18
(2,19)	1:693:A:ILE:HD13	1:696:A:ARG:HH11	14	2.54	1.27	2.18
(2,19)	1:693:A:ILE:HD13	1:696:A:ARG:HH21	14	2.54	1.27	2.18
(2,20)	1:693:A:ILE:HD11	1:696:A:ARG:HH21	14	2.54	1.27	2.18

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

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



9.5.2 Table : All distance violations [i](#)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	11	27.53
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	9	27.01
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	13	26.91
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	7	26.6
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	12	26.04
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	8	25.21
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	14	24.73
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	10	24.66
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	5	24.63
(1,1)	1:672:A:TRP:HE1	2:801:B:QOJ:H171	1	24.54

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

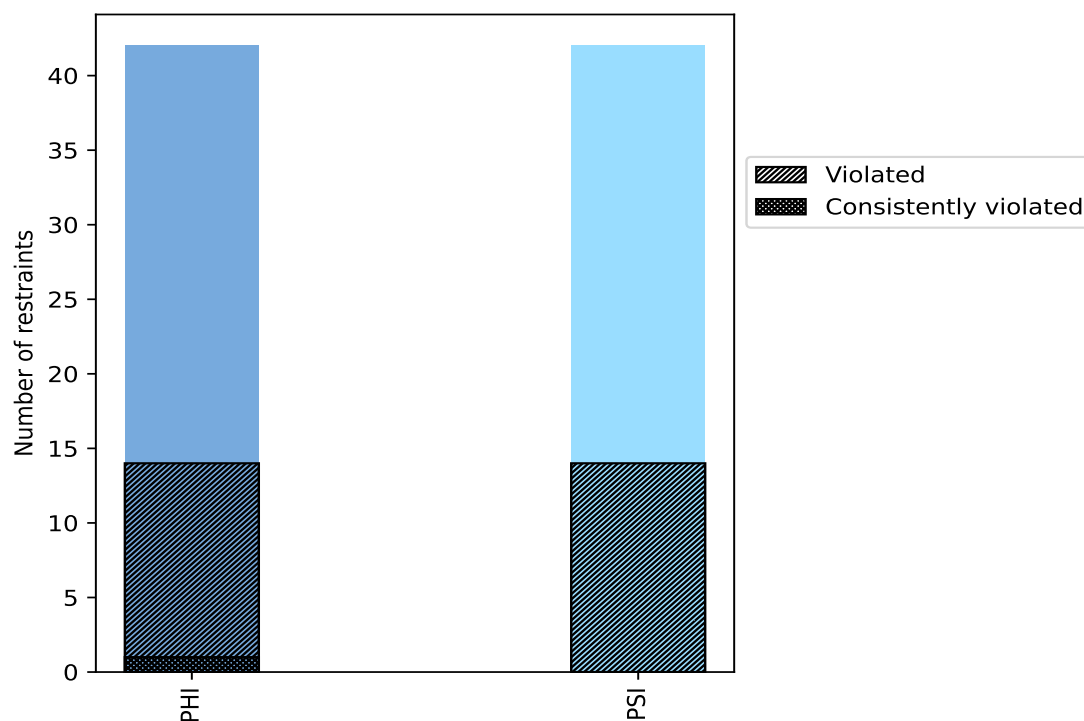
10.1 Summary of dihedral-angle violations [i](#)

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	42	50.0	14	33.3	16.7	1	2.4	1.2
PSI	42	50.0	14	33.3	16.7	0	0.0	0.0
Total	84	100.0	28	33.3	33.3	1	1.2	1.2

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](#)



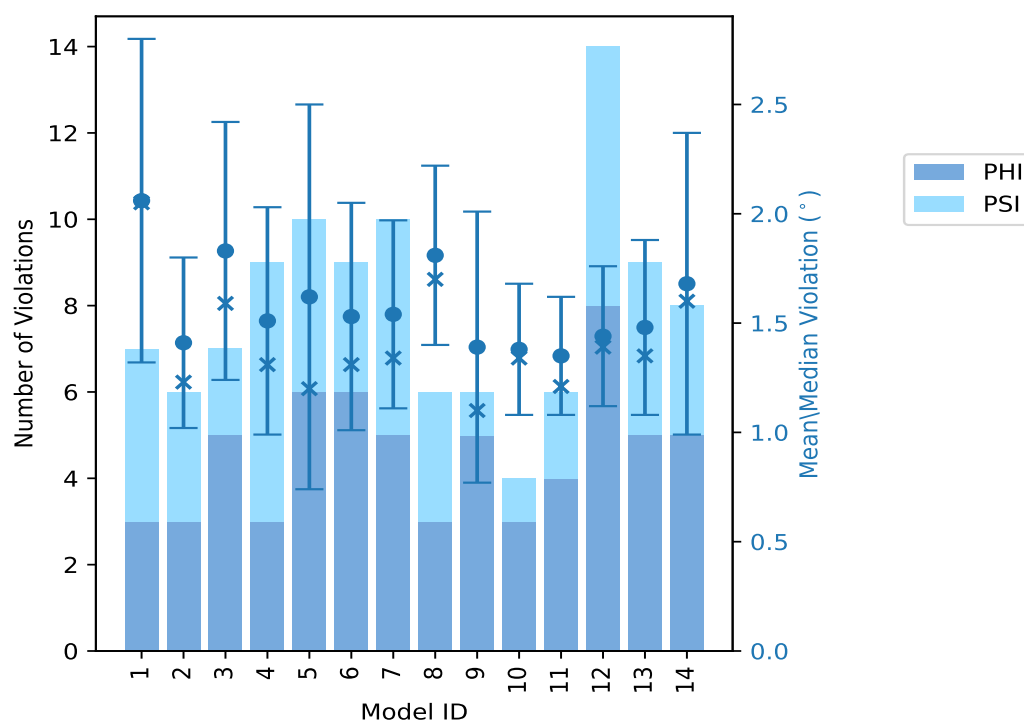
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	3	4	7	2.06	3.36	0.74	2.05
2	3	3	6	1.41	2.19	0.39	1.23
3	5	2	7	1.83	3.11	0.59	1.59
4	3	6	9	1.51	2.73	0.52	1.31
5	6	4	10	1.62	4.01	0.88	1.2
6	6	3	9	1.53	2.83	0.52	1.31
7	5	5	10	1.54	2.42	0.43	1.34
8	3	3	6	1.81	2.53	0.41	1.7
9	5	1	6	1.39	2.76	0.62	1.1
10	3	1	4	1.38	1.77	0.3	1.34
11	4	2	6	1.35	1.82	0.27	1.21
12	8	6	14	1.44	2.12	0.32	1.39
13	5	4	9	1.48	2.15	0.4	1.35
14	5	3	8	1.68	3.34	0.69	1.6

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

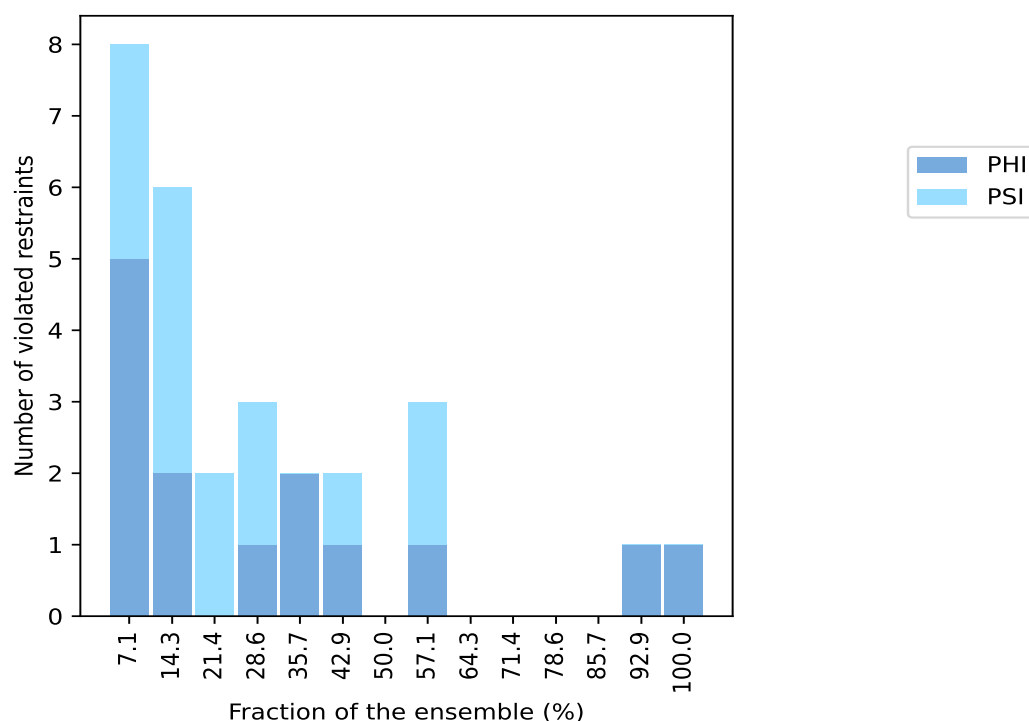
10.3 Dihedral-angle violation statistics for the ensemble

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	%
5	3	8	1	7.1
2	4	6	2	14.3
0	2	2	3	21.4
1	2	3	4	28.6
2	0	2	5	35.7
1	1	2	6	42.9
0	0	0	7	50.0
1	2	3	8	57.1
0	0	0	9	64.3
0	0	0	10	71.4
0	0	0	11	78.6
0	0	0	12	85.7
1	0	1	13	92.9
1	0	1	14	100.0

¹ Number of models with violations

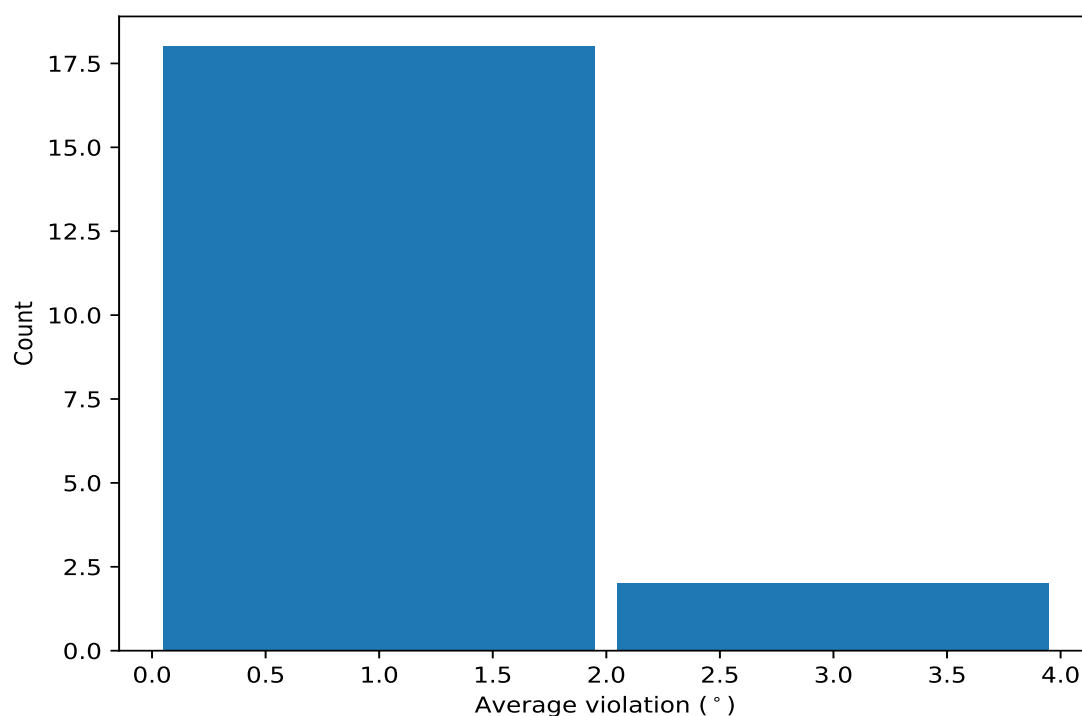
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

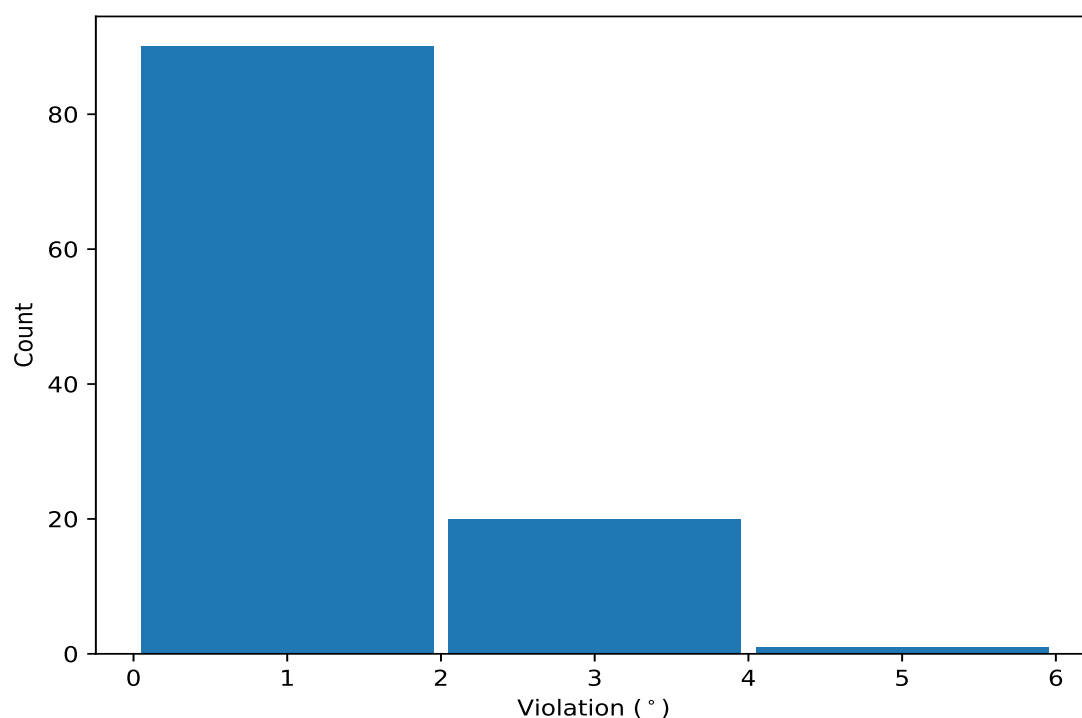
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	14	2.21	0.78	2.07
(1,47)	1:688:C:ILE:C	1:689:C:VAL:N	1:689:C:VAL:CA	1:689:C:VAL:C	13	1.51	0.35	1.44
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	8	2.25	0.72	2.0
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	8	1.84	0.54	1.89
(1,23)	1:674:C:ASP:C	1:675:C:ILE:N	1:675:C:ILE:CA	1:675:C:ILE:C	8	1.76	0.32	1.76
(1,62)	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1:698:C:VAL:N	6	1.45	0.3	1.44
(1,59)	1:695:C:LEU:C	1:696:C:ARG:N	1:696:C:ARG:CA	1:696:C:ARG:C	6	1.27	0.17	1.23
(1,21)	1:673:C:PHE:C	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	5	1.23	0.02	1.24
(1,19)	1:671:C:ASN:C	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	5	1.18	0.13	1.16
(1,20)	1:672:C:TRP:N	1:672:C:TRP:CA	1:672:C:TRP:C	1:673:C:PHE:N	4	1.5	0.17	1.44

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 (°)
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	5	4.01
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	1	3.36
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	14	3.34
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	3	3.11
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	6	2.83
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	9	2.76
(1,61)	1:696:C:ARG:C	1:697:C:ILE:N	1:697:C:ILE:CA	1:697:C:ILE:C	4	2.73
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	1	2.6
(1,22)	1:674:C:ASP:N	1:674:C:ASP:CA	1:674:C:ASP:C	1:675:C:ILE:N	8	2.53
(1,18)	1:671:C:ASN:N	1:671:C:ASN:CA	1:671:C:ASN:C	1:672:C:TRP:N	7	2.42