Full wwPDB NMR Structure Validation Report (i)

Jun 6, 2023 – 08:13 pm BST

PDB ID	:	7ZRU
BMRB ID	:	34732
Title	:	Solution structure of Pi6, a low affinity blocking kappa-K+-channel peptide from the scorpion Pandinus imperator
Authors	:	Delepierre, M.; Olamendi Portugal, T.; Possani, L.D.; Guijarro, J.I.
Deposited on	:	2022-05-05

This is a Full wwPDB NMR Structure Validation 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 (i)) were used in the production of this report:

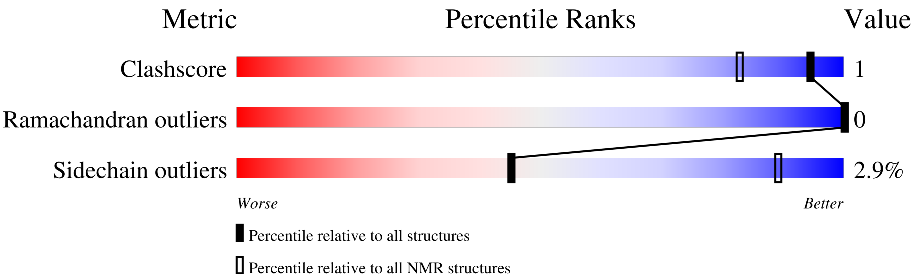
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 50%.

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	28	

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:3-A:22 (20)	0.55	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 2 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 402 atoms, of which 188 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Potassium channel toxin kappa-KTx 2.9.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	28	402	128	188	37	43	6	0

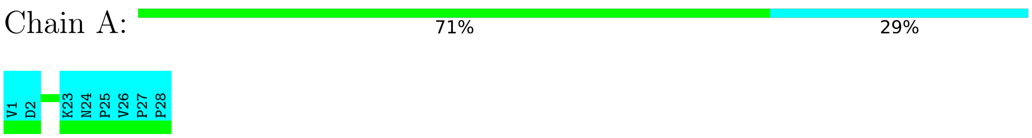
4 Residue-property plots (i)

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: Potassium channel toxin kappa-KTx 2.9

Chain A:



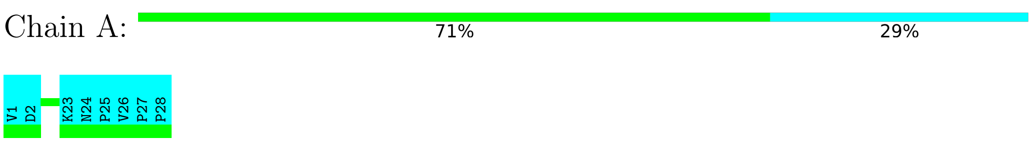
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Potassium channel toxin kappa-KTx 2.9

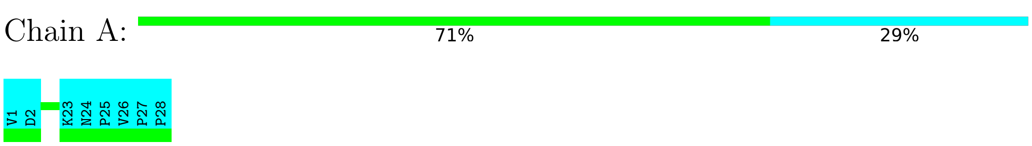
Chain A:



4.2.2 Score per residue for model 2

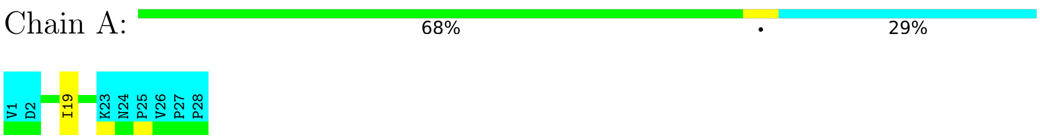
- Molecule 1: Potassium channel toxin kappa-KTx 2.9

Chain A:



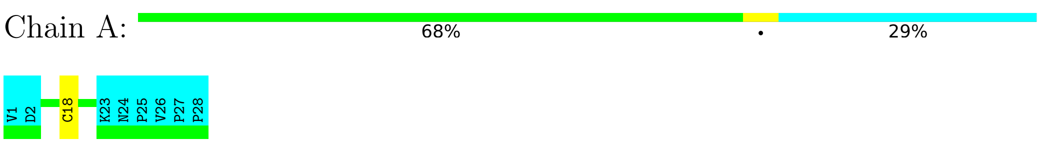
4.2.3 Score per residue for model 3

- Molecule 1: Potassium channel toxin kappa-KTx 2.9



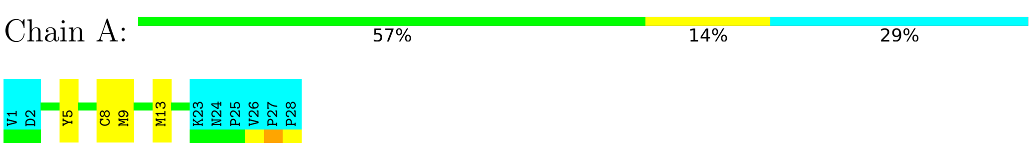
4.2.4 Score per residue for model 4

- Molecule 1: Potassium channel toxin kappa-KTx 2.9



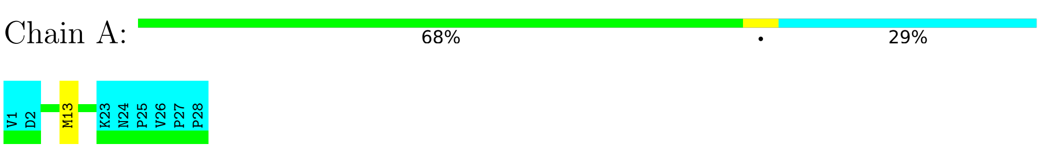
4.2.5 Score per residue for model 5

- Molecule 1: Potassium channel toxin kappa-KTx 2.9



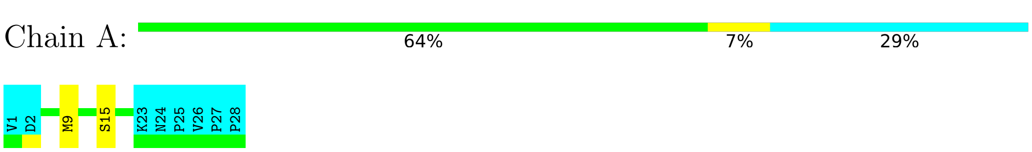
4.2.6 Score per residue for model 6

- Molecule 1: Potassium channel toxin kappa-KTx 2.9



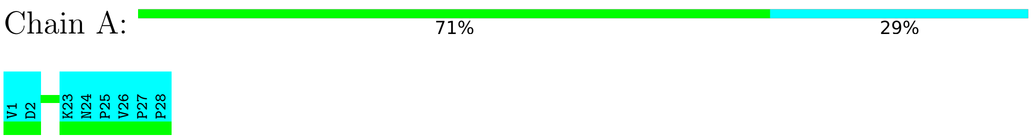
4.2.7 Score per residue for model 7

- Molecule 1: Potassium channel toxin kappa-KTx 2.9



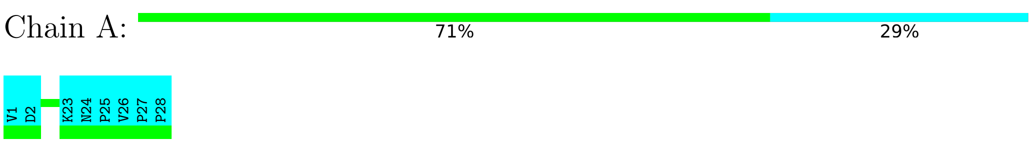
4.2.8 Score per residue for model 8

- Molecule 1: Potassium channel toxin kappa-KTx 2.9



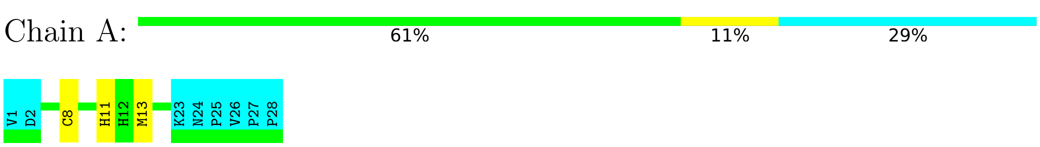
4.2.9 Score per residue for model 9

- Molecule 1: Potassium channel toxin kappa-KTx 2.9



4.2.10 Score per residue for model 10

- Molecule 1: Potassium channel toxin kappa-KTx 2.9



5 Refinement protocol and experimental data overview (i)

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

Of the 200 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
CNS	structure calculation	
ARIA	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	177
Number of shifts mapped to atoms	177
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	50%

6 Model quality (i)

6.1 Standard geometry (i)

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	153	124	121	0±0
All	All	1530	1240	1210	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:MET:SD	1:A:15:SER:HA	0.52	2.45	7	1
1:A:5:TYR:O	1:A:9:MET:HG3	0.48	2.09	5	1
1:A:8:CYS:HA	1:A:11:HIS:NE2	0.47	2.24	10	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	20/28 (71%)	19±1 (96±4%)	1±1 (4±4%)	0±0 (0±0%)	100	100
All	All	200/280 (71%)	191 (96%)	9 (4%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	17/25 (68%)	16±1 (97±4%)	0±1 (3±4%)	45	89
All	All	170/250 (68%)	165 (97%)	5 (3%)	45	89

All 3 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	13	MET	3
1	A	18	CYS	1
1	A	8	CYS	1

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 (i)

The completeness of assignment taking into account all chemical shift lists is 50% for the well-defined parts and 51% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *pi6cs.str*

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	177
Number of shifts mapped to atoms	177
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)

No chemical shift referencing corrections were calculated (not enough data).

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 50%, i.e. 116 atoms were assigned a chemical shift out of a possible 234. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**^{1}H**	**^{13}C**	**^{15}N**
Backbone	40/100 (40%)	40/40 (100%)	0/40 (0%)	0/20 (0%)
Sidechain	66/101 (65%)	66/66 (100%)	0/34 (0%)	0/1 (0%)
Aromatic	10/33 (30%)	10/16 (62%)	0/11 (0%)	0/6 (0%)
Overall	116/234 (50%)	116/122 (95%)	0/85 (0%)	0/27 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 51%, i.e. 174 atoms were assigned a chemical shift out of a possible 339. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	52/134 (39%)	52/53 (98%)	0/56 (0%)	0/25 (0%)
Sidechain	112/172 (65%)	112/112 (100%)	0/57 (0%)	0/3 (0%)
Aromatic	10/33 (30%)	10/16 (62%)	0/11 (0%)	0/6 (0%)
Overall	174/339 (51%)	174/181 (96%)	0/124 (0%)	0/34 (0%)

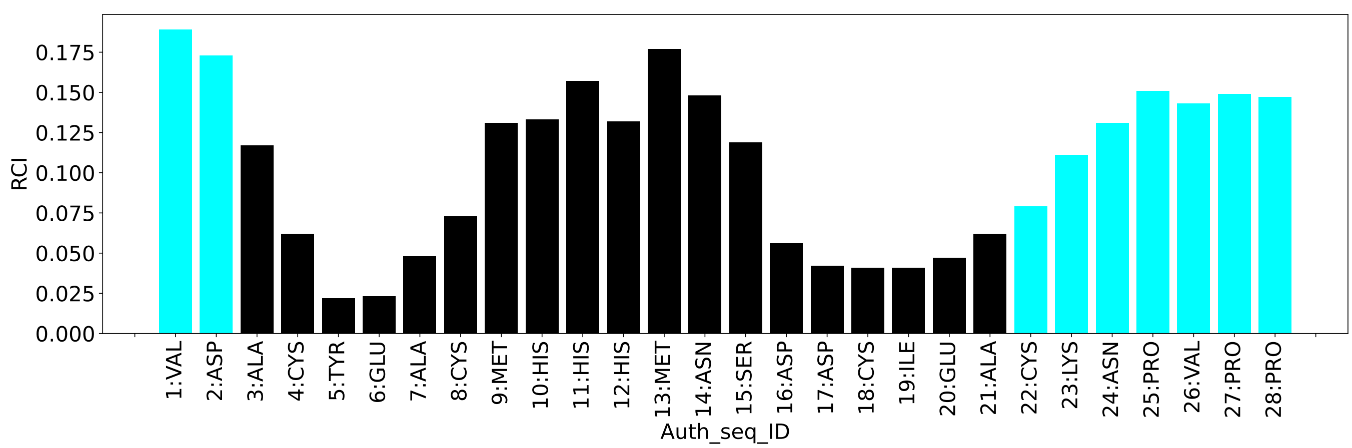
7.1.4 Statistically unusual chemical shifts ⓘ

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 (i)

8.1 Conformationally restricting restraints (i)

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	320
Intra-residue (|i-j|=0)	167
Sequential (|i-j|=1)	75
Medium range (|i-j|>1 and |i-j|<5)	46
Long range (|i-j|≥5)	21
Inter-chain	0
Hydrogen bond restraints	11
Disulfide bond restraints	0
Total dihedral-angle restraints	12
Number of unmapped restraints	0
Number of restraints per residue	11.9
Number of long range restraints per residue[1]	0.8

[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 (i)

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 (i)

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)	1.6	0.19
0.2-0.5 (Medium)	2.0	0.47
>0.5 (Large)	2.9	3.19

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)	0.2	1.2
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

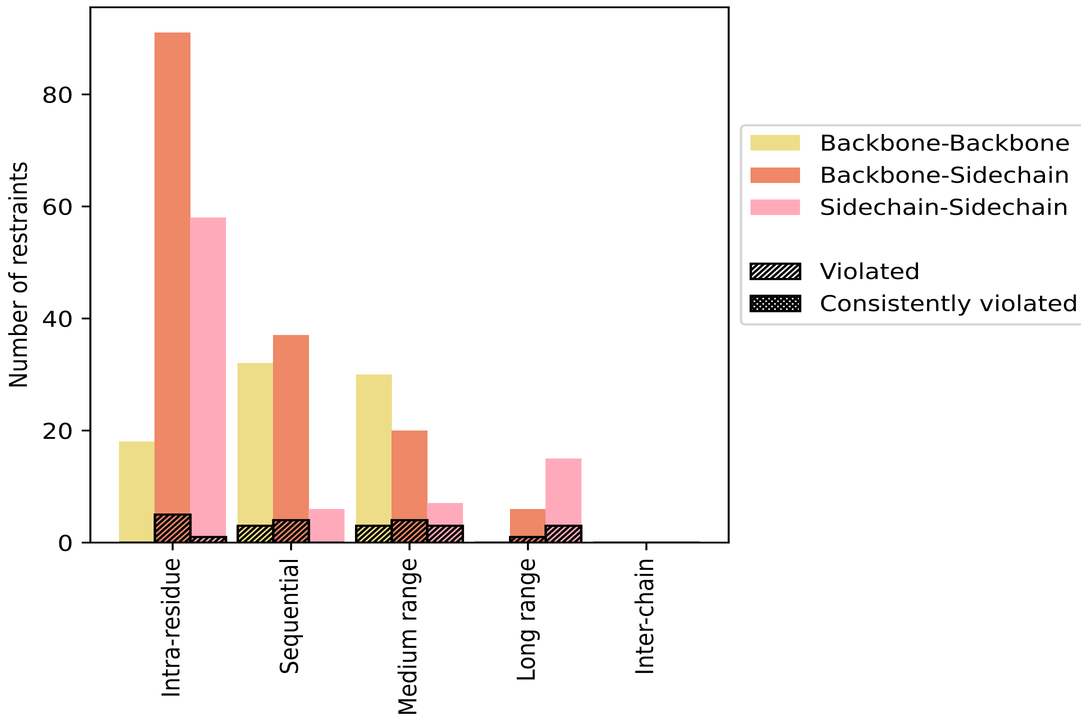
9.1 Summary of distance violations (i)

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)	167	52.2	6	3.6	1.9	0	0.0	0.0
Backbone-Backbone	18	5.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	91	28.4	5	5.5	1.6	0	0.0	0.0
Sidechain-Sidechain	58	18.1	1	1.7	0.3	0	0.0	0.0
Sequential (|i-j|=1)	75	23.4	7	9.3	2.2	0	0.0	0.0
Backbone-Backbone	32	10.0	3	9.4	0.9	0	0.0	0.0
Backbone-Sidechain	37	11.6	4	10.8	1.2	0	0.0	0.0
Sidechain-Sidechain	6	1.9	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	46	14.4	7	15.2	2.2	0	0.0	0.0
Backbone-Backbone	19	5.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	20	6.2	4	20.0	1.2	0	0.0	0.0
Sidechain-Sidechain	7	2.2	3	42.9	0.9	0	0.0	0.0
Long range (|i-j|≥5)	21	6.6	4	19.0	1.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	6	1.9	1	16.7	0.3	0	0.0	0.0
Sidechain-Sidechain	15	4.7	3	20.0	0.9	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	11	3.4	3	27.3	0.9	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	320	100.0	27	8.4	8.4	0	0.0	0.0
Backbone-Backbone	80	25.0	6	7.5	1.9	0	0.0	0.0
Backbone-Sidechain	154	48.1	14	9.1	4.4	0	0.0	0.0
Sidechain-Sidechain	86	26.9	7	8.1	2.2	0	0.0	0.0

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations (i)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model (i)

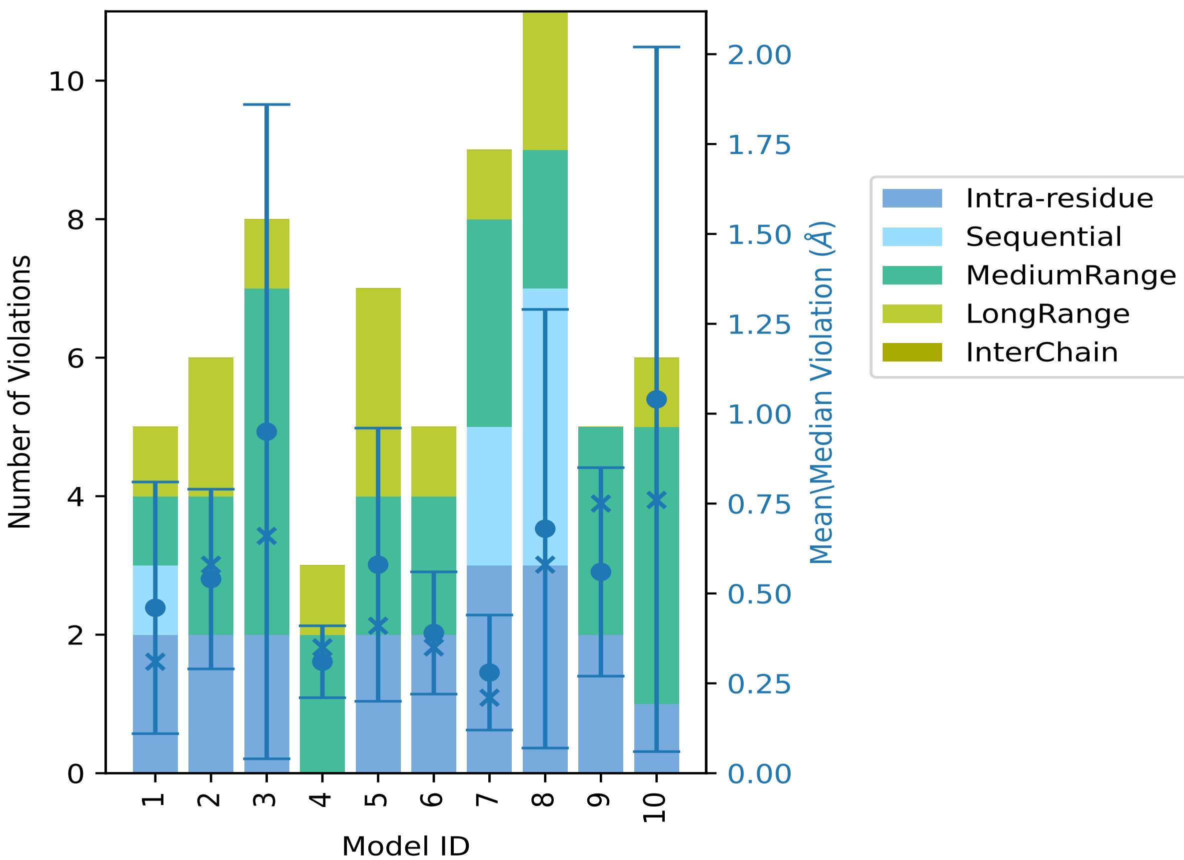
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

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	2	1	1	1	0	5	0.46	0.98	0.35	0.31
2	2	0	2	2	0	6	0.54	0.85	0.25	0.58
3	2	0	5	1	0	8	0.95	3.19	0.91	0.66
4	0	0	2	1	0	3	0.31	0.41	0.1	0.35
5	2	0	2	3	0	7	0.58	1.3	0.38	0.41
6	2	0	2	1	0	5	0.39	0.61	0.17	0.35
7	3	2	3	1	0	9	0.28	0.62	0.16	0.21
8	3	4	2	2	0	11	0.68	2.3	0.61	0.58
9	2	0	3	0	0	5	0.56	0.82	0.29	0.75
10	1	0	4	1	0	6	1.04	3.13	0.98	0.76

[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 (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, 285(IR:161, SQ:68, MR:39, LR:17, 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	7	2	2	0	12	1	10.0
1	0	0	0	0	1	2	20.0
2	0	3	0	0	5	3	30.0
1	0	0	0	0	1	4	40.0

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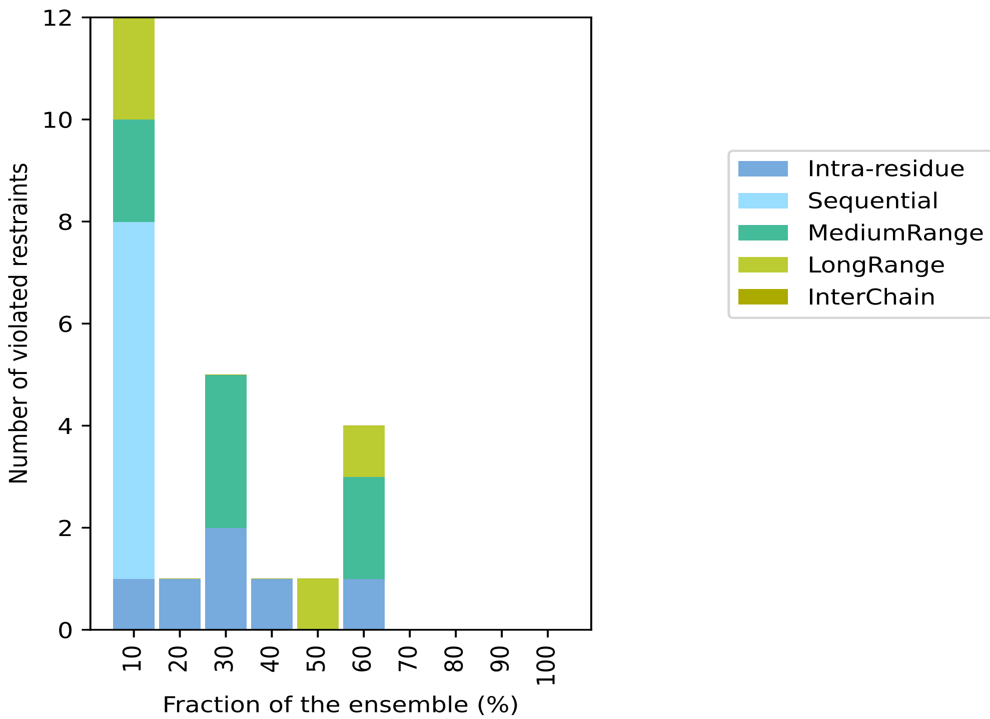
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	1	0	1	5	50.0
1	0	2	1	0	4	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	0	0	0	8	80.0
0	0	0	0	0	0	9	90.0
0	0	0	0	0	0	10	100.0

[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

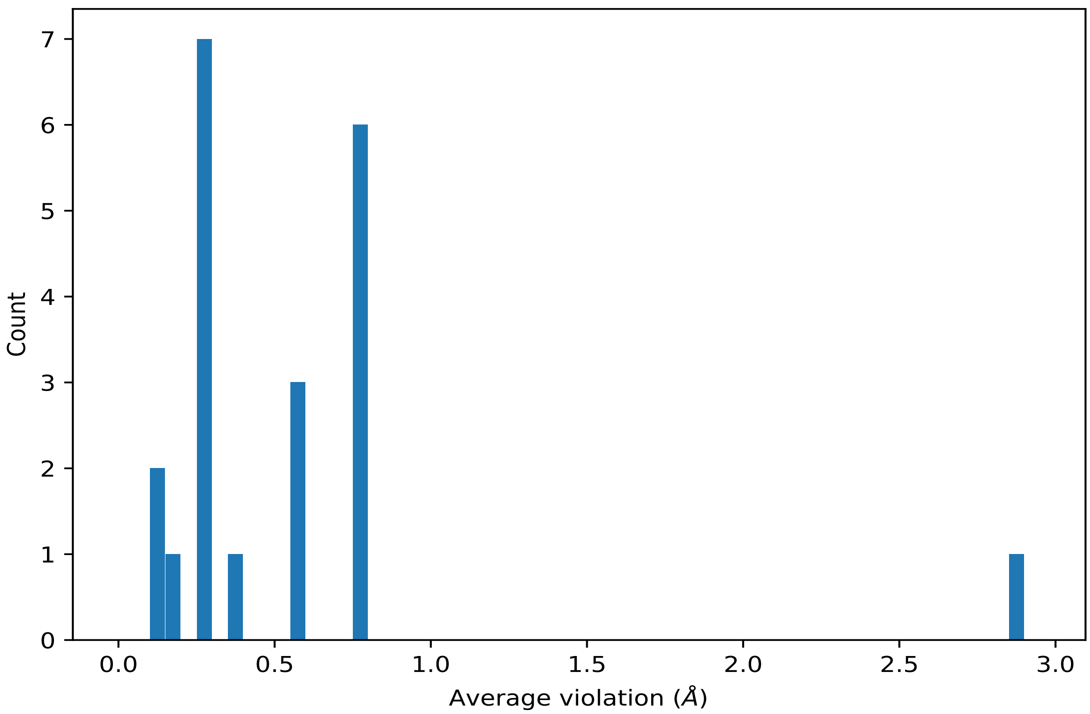
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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 violation for each restraint sorted by number of violated models and the mean 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)
(3,159)	1:A:9:MET:HB3	1:A:6:GLU:HA	6	0.77	0.3	0.69
(3,154)	1:A:22:CYS:HB3	1:A:19:ILE:HA	6	0.75	0.14	0.74
(3,198)	1:A:9:MET:HE2	1:A:15:SER:HB2	6	0.59	0.4	0.42
(3,198)	1:A:9:MET:HE1	1:A:15:SER:HB2	6	0.59	0.4	0.42
(3,198)	1:A:9:MET:HE3	1:A:15:SER:HB2	6	0.59	0.4	0.42
(3,100)	1:A:9:MET:H	1:A:9:MET:HB3	6	0.38	0.03	0.4
(3,197)	1:A:9:MET:HE2	1:A:15:SER:HB3	5	0.75	0.33	0.58
(3,197)	1:A:9:MET:HE1	1:A:15:SER:HB3	5	0.75	0.33	0.58
(3,197)	1:A:9:MET:HE3	1:A:15:SER:HB3	5	0.75	0.33	0.58
(3,76)	1:A:16:ASP:H	1:A:16:ASP:HB3	4	0.76	0.01	0.76
(3,16)	1:A:12:HIS:HD2	1:A:8:CYS:HA	3	2.87	0.41	3.13
(3,90)	1:A:5:TYR:HE1	1:A:9:MET:HE2	3	0.26	0.08	0.27
(3,90)	1:A:5:TYR:HE1	1:A:9:MET:HE1	3	0.26	0.08	0.27
(3,90)	1:A:5:TYR:HE1	1:A:9:MET:HE3	3	0.26	0.08	0.27
(3,90)	1:A:5:TYR:HE2	1:A:9:MET:HE2	3	0.26	0.08	0.27
(3,90)	1:A:5:TYR:HE2	1:A:9:MET:HE1	3	0.26	0.08	0.27

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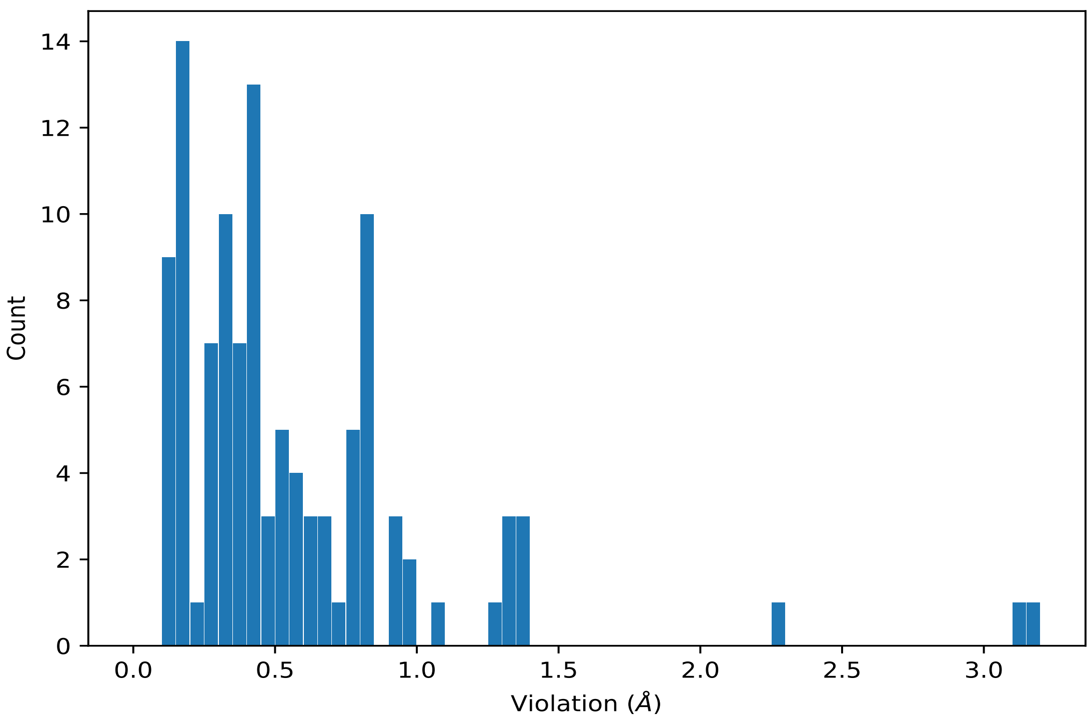
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,90)	1:A:5:TYR:HE2	1:A:9:MET:HE3	3	0.26	0.08	0.27
(3,220)	1:A:2:ASP:HB2	1:A:5:TYR:HB3	3	0.25	0.05	0.27
(3,51)	1:A:12:HIS:HD2	1:A:12:HIS:HB2	3	0.16	0.0	0.16
(3,32)	1:A:15:SER:H	1:A:15:SER:HB2	3	0.11	0.0	0.11
(3,60)	1:A:22:CYS:H	1:A:22:CYS:HB3	2	0.13	0.0	0.13

[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 lists the absolute value of the violation for each restraint in the ensemble sorted by its 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)
(3,16)	1:A:12:HIS:HD2	1:A:8:CYS:HA	3	3.19
(3,16)	1:A:12:HIS:HD2	1:A:8:CYS:HA	10	3.13
(3,16)	1:A:12:HIS:HD2	1:A:8:CYS:HA	8	2.3
(3,198)	1:A:9:MET:HE2	1:A:15:SER:HB2	8	1.37
(3,198)	1:A:9:MET:HE1	1:A:15:SER:HB2	8	1.37
(3,198)	1:A:9:MET:HE3	1:A:15:SER:HB2	8	1.37
(3,197)	1:A:9:MET:HE2	1:A:15:SER:HB3	5	1.3
(3,197)	1:A:9:MET:HE1	1:A:15:SER:HB3	5	1.3
(3,197)	1:A:9:MET:HE3	1:A:15:SER:HB3	5	1.3
(3,159)	1:A:9:MET:HB3	1:A:6:GLU:HA	3	1.29
(2,1)	1:A:2:ASP:O	1:A:6:GLU:H	10	1.06
(3,154)	1:A:22:CYS:HB3	1:A:19:ILE:HA	1	0.98
(3,159)	1:A:9:MET:HB3	1:A:6:GLU:HA	5	0.97
(3,197)	1:A:9:MET:HE2	1:A:15:SER:HB3	3	0.95
(3,197)	1:A:9:MET:HE1	1:A:15:SER:HB3	3	0.95
(3,197)	1:A:9:MET:HE3	1:A:15:SER:HB3	3	0.95
(3,198)	1:A:9:MET:HE2	1:A:15:SER:HB2	2	0.85
(3,198)	1:A:9:MET:HE1	1:A:15:SER:HB2	2	0.85
(3,198)	1:A:9:MET:HE3	1:A:15:SER:HB2	2	0.85
(3,154)	1:A:22:CYS:HB3	1:A:19:ILE:HA	10	0.84
(1,37)	1:A:19:ILE:HG22	1:A:23:LYS:HE3	9	0.82
(1,37)	1:A:19:ILE:HG21	1:A:23:LYS:HE3	9	0.82
(1,37)	1:A:19:ILE:HG23	1:A:23:LYS:HE3	9	0.82
(1,37)	1:A:19:ILE:HG22	1:A:23:LYS:HE2	9	0.82
(1,37)	1:A:19:ILE:HG21	1:A:23:LYS:HE2	9	0.82
(1,37)	1:A:19:ILE:HG23	1:A:23:LYS:HE2	9	0.82
(3,154)	1:A:22:CYS:HB3	1:A:19:ILE:HA	9	0.78
(3,76)	1:A:16:ASP:H	1:A:16:ASP:HB3	2	0.77
(3,76)	1:A:16:ASP:H	1:A:16:ASP:HB3	1	0.76
(3,76)	1:A:16:ASP:H	1:A:16:ASP:HB3	3	0.75
(3,76)	1:A:16:ASP:H	1:A:16:ASP:HB3	9	0.75
(3,159)	1:A:9:MET:HB3	1:A:6:GLU:HA	8	0.71
(3,154)	1:A:22:CYS:HB3	1:A:19:ILE:HA	2	0.7
(3,42)	1:A:5:TYR:H	1:A:4:CYS:HB3	8	0.68
(3,159)	1:A:9:MET:HB3	1:A:6:GLU:HA	10	0.67
(3,159)	1:A:9:MET:HB3	1:A:6:GLU:HA	7	0.62
(3,52)	1:A:4:CYS:H	1:A:4:CYS:HB2	8	0.61
(3,154)	1:A:22:CYS:HB3	1:A:19:ILE:HA	6	0.61
(3,197)	1:A:9:MET:HE2	1:A:15:SER:HB3	8	0.58
(3,197)	1:A:9:MET:HE1	1:A:15:SER:HB3	8	0.58
(3,197)	1:A:9:MET:HE3	1:A:15:SER:HB3	8	0.58
(3,154)	1:A:22:CYS:HB3	1:A:19:ILE:HA	3	0.57
(3,197)	1:A:9:MET:HE2	1:A:15:SER:HB3	6	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,197)	1:A:9:MET:HE1	1:A:15:SER:HB3	6	0.53
(3,197)	1:A:9:MET:HE3	1:A:15:SER:HB3	6	0.53
(1,52)	1:A:18:CYS:HB3	1:A:8:CYS:HB2	5	0.52
(1,52)	1:A:18:CYS:HB3	1:A:8:CYS:HB3	5	0.52
(3,206)	1:A:9:MET:HE2	1:A:15:SER:HA	2	0.47
(3,206)	1:A:9:MET:HE1	1:A:15:SER:HA	2	0.47
(3,206)	1:A:9:MET:HE3	1:A:15:SER:HA	2	0.47
(3,198)	1:A:9:MET:HE2	1:A:15:SER:HB2	7	0.44
(3,198)	1:A:9:MET:HE1	1:A:15:SER:HB2	7	0.44
(3,198)	1:A:9:MET:HE3	1:A:15:SER:HB2	7	0.44
(3,197)	1:A:9:MET:HE2	1:A:15:SER:HB3	4	0.41
(3,197)	1:A:9:MET:HE1	1:A:15:SER:HB3	4	0.41
(3,197)	1:A:9:MET:HE3	1:A:15:SER:HB3	4	0.41
(3,100)	1:A:9:MET:H	1:A:9:MET:HB3	3	0.41
(3,100)	1:A:9:MET:H	1:A:9:MET:HB3	5	0.41
(3,198)	1:A:9:MET:HE2	1:A:15:SER:HB2	5	0.4
(3,198)	1:A:9:MET:HE1	1:A:15:SER:HB2	5	0.4
(3,198)	1:A:9:MET:HE3	1:A:15:SER:HB2	5	0.4
(3,100)	1:A:9:MET:H	1:A:9:MET:HB3	7	0.4
(3,100)	1:A:9:MET:H	1:A:9:MET:HB3	8	0.4
(3,141)	1:A:25:PRO:HD2	1:A:24:ASN:HA	8	0.39
(3,90)	1:A:5:TYR:HE1	1:A:9:MET:HE2	2	0.36
(3,90)	1:A:5:TYR:HE1	1:A:9:MET:HE1	2	0.36
(3,90)	1:A:5:TYR:HE1	1:A:9:MET:HE3	2	0.36
(3,90)	1:A:5:TYR:HE2	1:A:9:MET:HE2	2	0.36
(3,90)	1:A:5:TYR:HE2	1:A:9:MET:HE1	2	0.36
(3,90)	1:A:5:TYR:HE2	1:A:9:MET:HE3	2	0.36
(3,100)	1:A:9:MET:H	1:A:9:MET:HB3	6	0.35
(2,7)	1:A:8:CYS:O	1:A:12:HIS:H	4	0.35
(3,159)	1:A:9:MET:HB3	1:A:6:GLU:HA	6	0.34
(3,100)	1:A:9:MET:H	1:A:9:MET:HB3	10	0.34
(1,40)	1:A:23:LYS:HD2	1:A:20:GLU:HA	9	0.33
(1,40)	1:A:23:LYS:HD3	1:A:20:GLU:HA	9	0.33
(3,220)	1:A:2:ASP:HB2	1:A:5:TYR:HB3	3	0.31
(3,198)	1:A:9:MET:HE2	1:A:15:SER:HB2	1	0.31
(3,198)	1:A:9:MET:HE1	1:A:15:SER:HB2	1	0.31
(3,198)	1:A:9:MET:HE3	1:A:15:SER:HB2	1	0.31
(3,90)	1:A:5:TYR:HE1	1:A:9:MET:HE2	7	0.27
(3,90)	1:A:5:TYR:HE1	1:A:9:MET:HE1	7	0.27
(3,90)	1:A:5:TYR:HE1	1:A:9:MET:HE3	7	0.27
(3,90)	1:A:5:TYR:HE2	1:A:9:MET:HE2	7	0.27
(3,90)	1:A:5:TYR:HE2	1:A:9:MET:HE1	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,90)	1:A:5:TYR:HE2	1:A:9:MET:HE3	7	0.27
(3,220)	1:A:2:ASP:HB2	1:A:5:TYR:HB3	5	0.27
(3,238)	1:A:14:ASN:H	1:A:13:MET:HB2	7	0.21
(3,198)	1:A:9:MET:HE2	1:A:15:SER:HB2	10	0.19
(3,198)	1:A:9:MET:HE1	1:A:15:SER:HB2	10	0.19
(3,198)	1:A:9:MET:HE3	1:A:15:SER:HB2	10	0.19
(3,220)	1:A:2:ASP:HB2	1:A:5:TYR:HB3	7	0.18
(3,139)	1:A:23:LYS:H	1:A:22:CYS:H	8	0.17
(2,5)	1:A:7:ALA:O	1:A:10:HIS:H	4	0.17
(3,90)	1:A:5:TYR:HE1	1:A:9:MET:HE2	3	0.16
(3,90)	1:A:5:TYR:HE1	1:A:9:MET:HE1	3	0.16
(3,90)	1:A:5:TYR:HE1	1:A:9:MET:HE3	3	0.16
(3,90)	1:A:5:TYR:HE2	1:A:9:MET:HE2	3	0.16
(3,90)	1:A:5:TYR:HE2	1:A:9:MET:HE1	3	0.16
(3,90)	1:A:5:TYR:HE2	1:A:9:MET:HE3	3	0.16
(3,51)	1:A:12:HIS:HD2	1:A:12:HIS:HB2	5	0.16
(3,51)	1:A:12:HIS:HD2	1:A:12:HIS:HB2	7	0.16
(3,51)	1:A:12:HIS:HD2	1:A:12:HIS:HB2	8	0.15
(3,8)	1:A:26:VAL:H	1:A:25:PRO:HA	7	0.13
(3,60)	1:A:22:CYS:H	1:A:22:CYS:HB3	1	0.13
(3,60)	1:A:22:CYS:H	1:A:22:CYS:HB3	6	0.13
(3,32)	1:A:15:SER:H	1:A:15:SER:HB2	2	0.12
(3,32)	1:A:15:SER:H	1:A:15:SER:HB2	7	0.11
(3,32)	1:A:15:SER:H	1:A:15:SER:HB2	9	0.11
(3,17)	1:A:24:ASN:H	1:A:23:LYS:HA	1	0.11
(3,140)	1:A:25:PRO:HD3	1:A:24:ASN:HA	8	0.11

10 Dihedral-angle violation analysis (i)

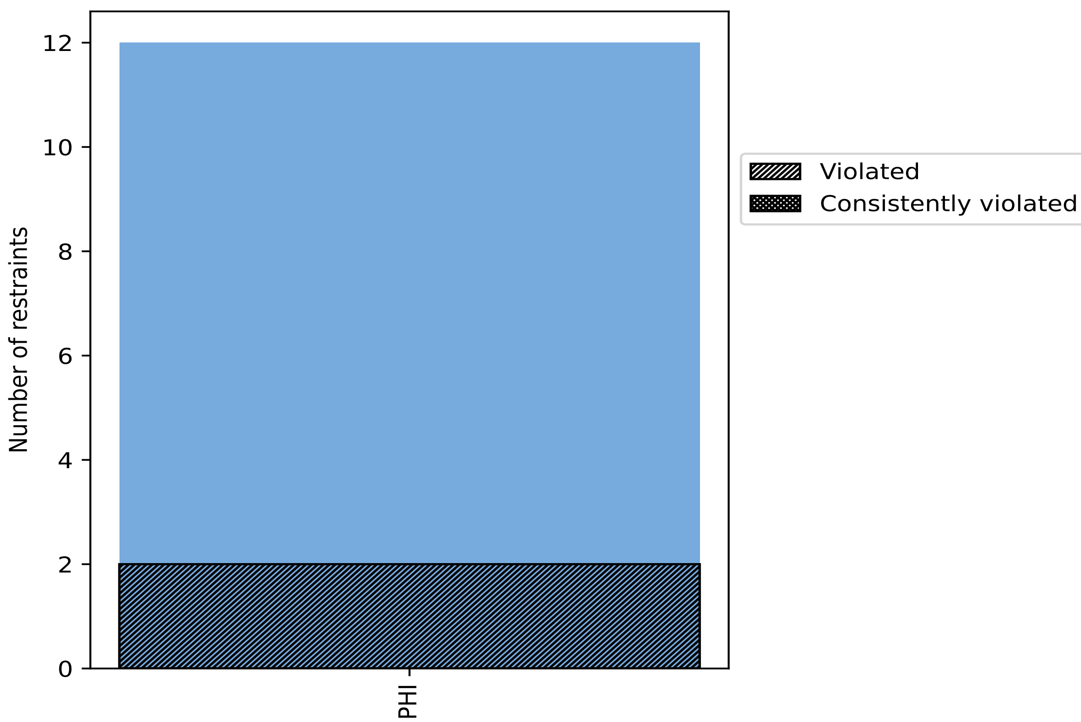
10.1 Summary of dihedral-angle violations (i)

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	12	100.0	2	16.7	16.7	0	0.0	0.0
Total	12	100.0	2	16.7	16.7	0	0.0	0.0

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations (i)



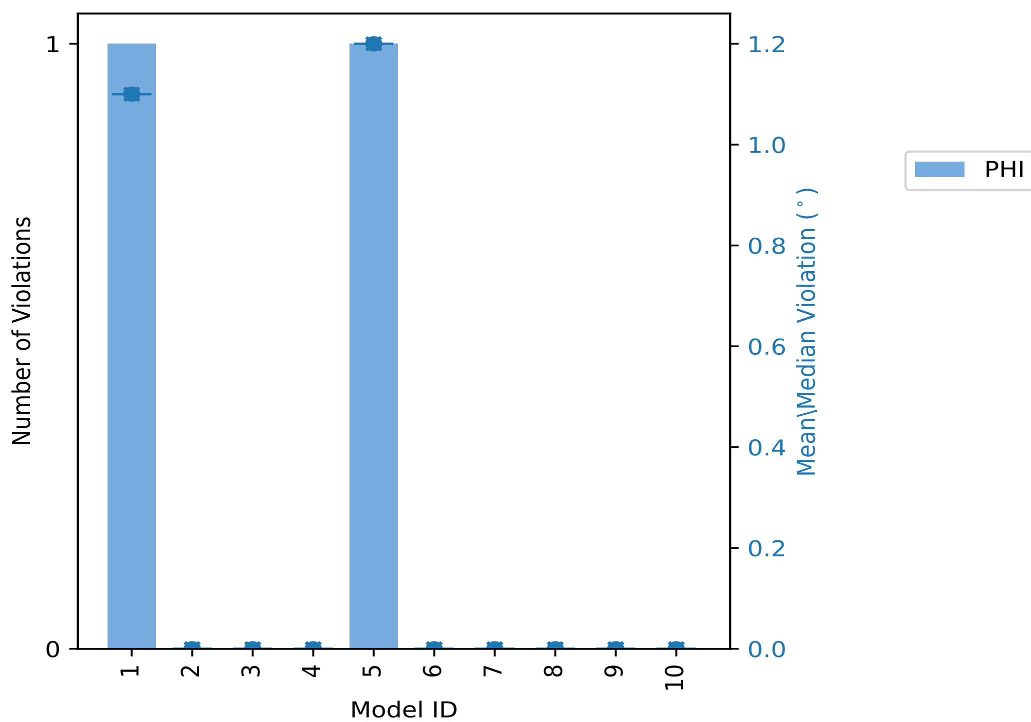
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations		Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	Total				
1	1	1	1.1	1.1	0.0	1.1
2	0	0	0.0	0.0	0.0	0.0
3	0	0	0.0	0.0	0.0	0.0
4	0	0	0.0	0.0	0.0	0.0
5	1	1	1.2	1.2	0.0	1.2
6	0	0	0.0	0.0	0.0	0.0
7	0	0	0.0	0.0	0.0	0.0
8	0	0	0.0	0.0	0.0	0.0
9	0	0	0.0	0.0	0.0	0.0
10	0	0	0.0	0.0	0.0	0.0

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

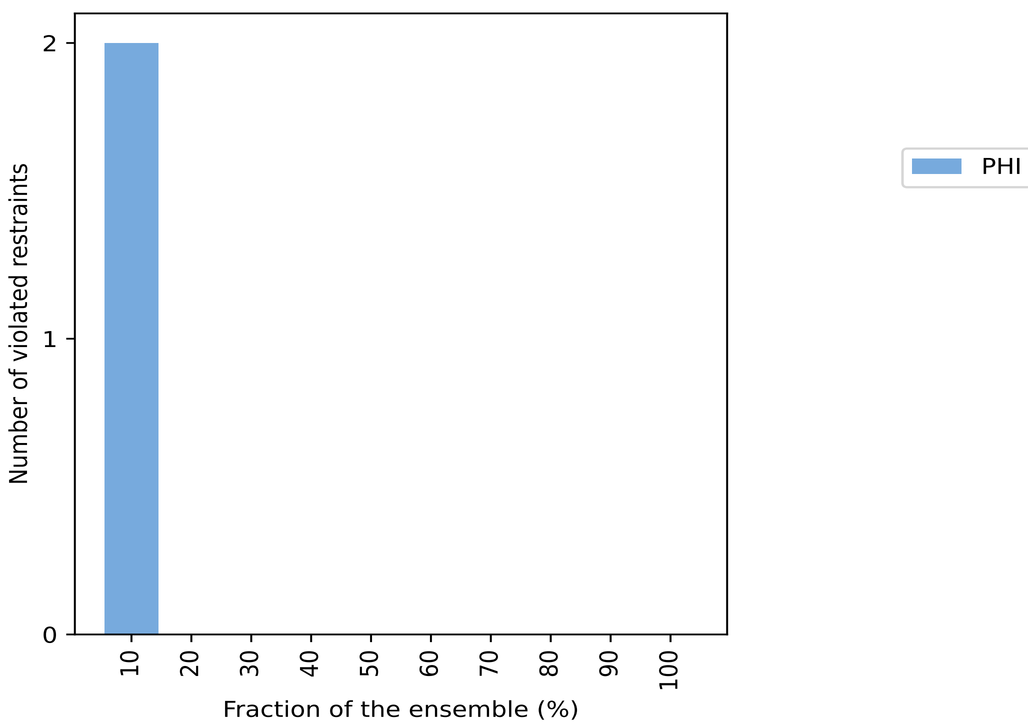
10.3 Dihedral-angle violation statistics for the ensemble (i)

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	Total	Count[1]	%
2	2	1	10.0
0	0	2	20.0
0	0	3	30.0
0	0	4	40.0
0	0	5	50.0
0	0	6	60.0
0	0	7	70.0
0	0	8	80.0
0	0	9	90.0
0	0	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)

No violations found

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.
Data insufficient to plot histogram

10.5.2 Table: All violated dihedral-angle restraints (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its 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 (°)
(1,9)	1:A:19:ILE:C	1:A:20:GLU:N	1:A:20:GLU:CA	1:A:20:GLU:C	5	1.2
(1,6)	1:A:10:HIS:C	1:A:11:HIS:N	1:A:11:HIS:CA	1:A:11:HIS:C	1	1.1