Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 08:45 PM EDT

PDB ID	:	2MXM
BMRB ID	:	25419
Title	:	NMR solution structure of TRTX-Tp1a from the tarantula Thrixopelma pruriens
Authors	:	Rosengren, K.
Deposited on	:	2015-01-08

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:

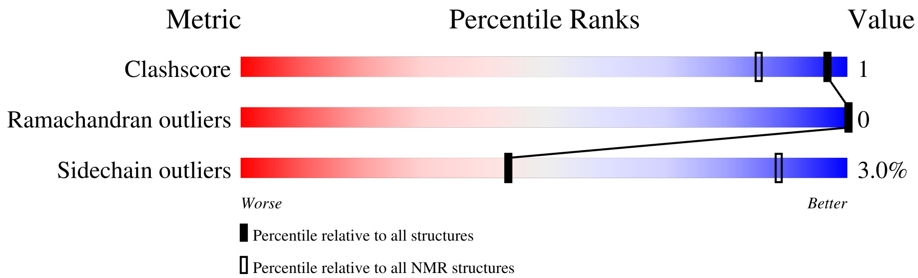
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

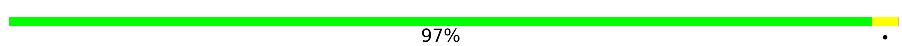
The overall completeness of chemical shifts assignment is 51%.

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	33	

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *best molprobity score*.

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:33 (33)	0.68	17

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 5 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 512 atoms, of which 249 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called entity.

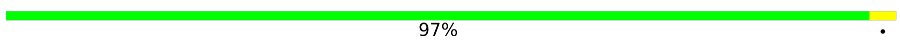
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	33	512	162	249	51	44	6	0

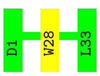
4 Residue-property plots (i)

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: entity

Chain A:


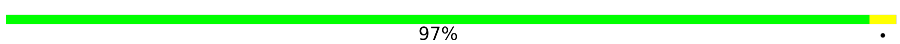


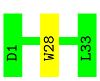
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

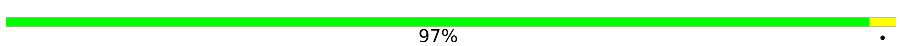
- Molecule 1: entity

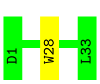
Chain A:




4.2.2 Score per residue for model 2

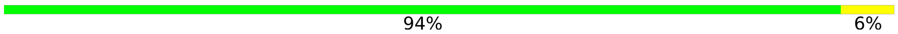
- Molecule 1: entity

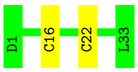
Chain A:




4.2.3 Score per residue for model 3

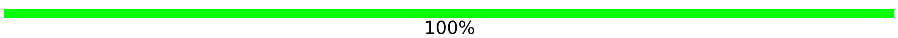
- Molecule 1: entity

Chain A: 



4.2.4 Score per residue for model 4

- Molecule 1: entity

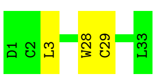
Chain A: 

There are no outlier residues in this chain.

4.2.5 Score per residue for model 5

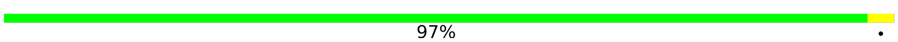
- Molecule 1: entity

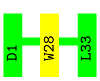
Chain A: 



4.2.6 Score per residue for model 6

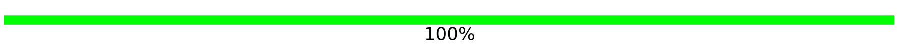
- Molecule 1: entity

Chain A: 



4.2.7 Score per residue for model 7

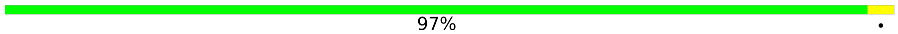
- Molecule 1: entity

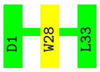
Chain A: 

There are no outlier residues in this chain.

4.2.8 Score per residue for model 8

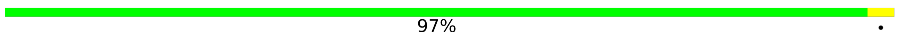
• Molecule 1: entity

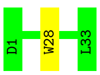
Chain A: 



4.2.9 Score per residue for model 9

• Molecule 1: entity

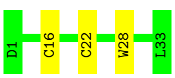
Chain A: 



4.2.10 Score per residue for model 10

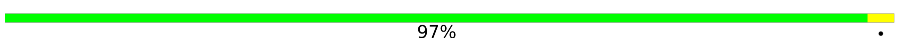
• Molecule 1: entity

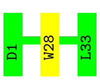
Chain A: 



4.2.11 Score per residue for model 11

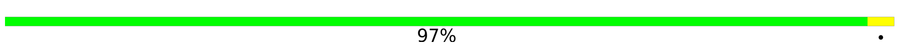
• Molecule 1: entity

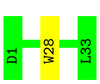
Chain A: 



4.2.12 Score per residue for model 12

• Molecule 1: entity

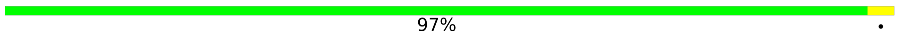
Chain A: 

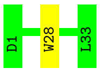


4.2.13 Score per residue for model 13

• Molecule 1: entity

Chain A:

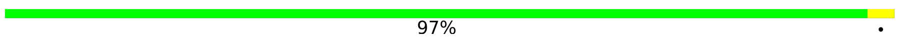


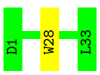


4.2.14 Score per residue for model 14

• Molecule 1: entity

Chain A:

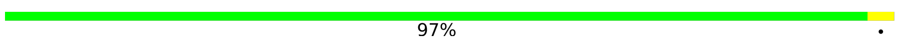


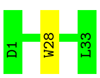


4.2.15 Score per residue for model 15

• Molecule 1: entity

Chain A:

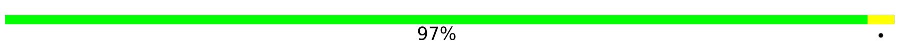


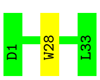


4.2.16 Score per residue for model 16

• Molecule 1: entity

Chain A:

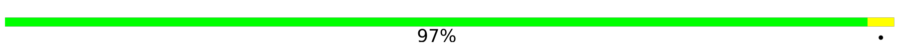


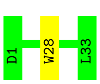


4.2.17 Score per residue for model 17 (medoid)

• Molecule 1: entity

Chain A:

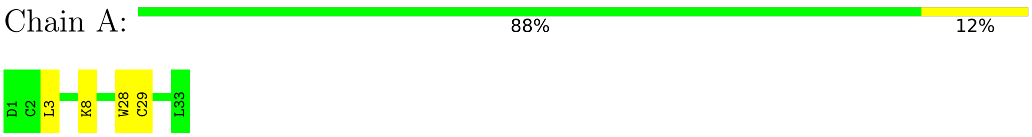




4.2.18 Score per residue for model 18

- Molecule 1: entity

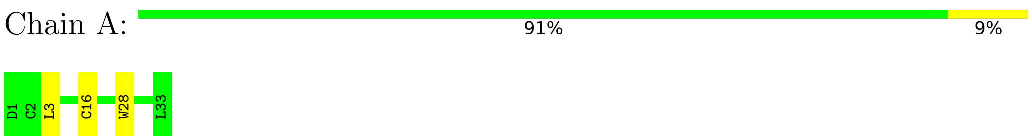
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: entity

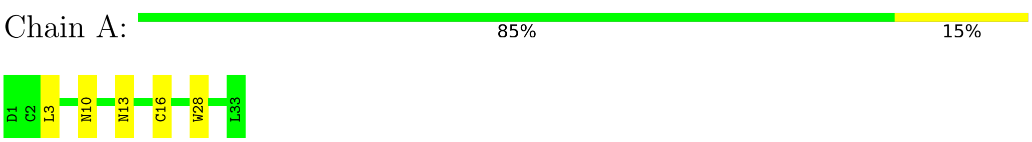
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: entity

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	
CNS	refinement	1.2

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	225
Number of shifts mapped to atoms	225
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	51%

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	263	249	249	0±1
All	All	5260	4980	4980	7

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:3:LEU:HB2	1:A:16:CYS:SG	0.67	2.29	20	2
1:A:16:CYS:SG	1:A:22:CYS:HB2	0.49	2.47	10	2
1:A:3:LEU:HB2	1:A:29:CYS:SG	0.47	2.49	5	2
1:A:10:ASN:HB2	1:A:13:ASN:O	0.47	2.09	20	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	31/33 (94%)	30±1 (98±2%)	1±1 (2±2%)	0±0 (0±0%)	100	100
All	All	620/660 (94%)	609 (98%)	11 (2%)	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	30/30 (100%)	29±0 (97±1%)	1±0 (3±1%)	44	89
All	All	600/600 (100%)	582 (97%)	18 (3%)	44	89

All 2 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	28	TRP	17
1	A	8	LYS	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 51% 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: *assigned_chem_shift_list_1*

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	225
Number of shifts mapped to atoms	225
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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 51%, i.e. 222 atoms were assigned a chemical shift out of a possible 433. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}**H**	^{13}**C**	^{15}**N**
Backbone	67/166 (40%)	67/68 (99%)	0/66 (0%)	0/32 (0%)
Sidechain	135/219 (62%)	135/139 (97%)	0/68 (0%)	0/12 (0%)
Aromatic	20/48 (42%)	20/25 (80%)	0/19 (0%)	0/4 (0%)
Overall	222/433 (51%)	222/232 (96%)	0/153 (0%)	0/48 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 51%, i.e. 222 atoms were assigned a chemical shift out of a possible 433. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	67/166 (40%)	67/68 (99%)	0/66 (0%)	0/32 (0%)
Sidechain	135/219 (62%)	135/139 (97%)	0/68 (0%)	0/12 (0%)
Aromatic	20/48 (42%)	20/25 (80%)	0/19 (0%)	0/4 (0%)
Overall	222/433 (51%)	222/232 (96%)	0/153 (0%)	0/48 (0%)

7.1.4 Statistically unusual chemical shifts (i)

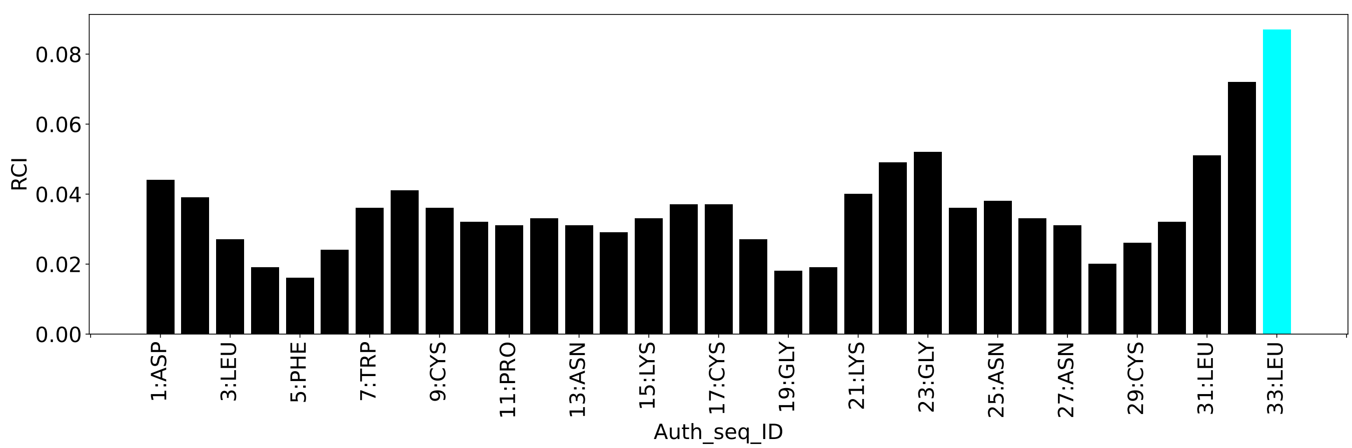
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	4	LYS	HB2	0.06	0.58 – 2.97	-7.2

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 (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	369
Intra-residue (|i-j|=0)	168
Sequential (|i-j|=1)	100
Medium range (|i-j|>1 and |i-j|<5)	35
Long range (|i-j|≥5)	46
Inter-chain	0
Hydrogen bond restraints	20
Disulfide bond restraints	0
Total dihedral-angle restraints	37
Number of unmapped restraints	0
Number of restraints per residue	12.3
Number of long range restraints per residue[1]	1.8

[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)	1.2	0.2
0.2-0.5 (Medium)	1.3	0.37
>0.5 (Large)	None	None

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)	0.3	1.9
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

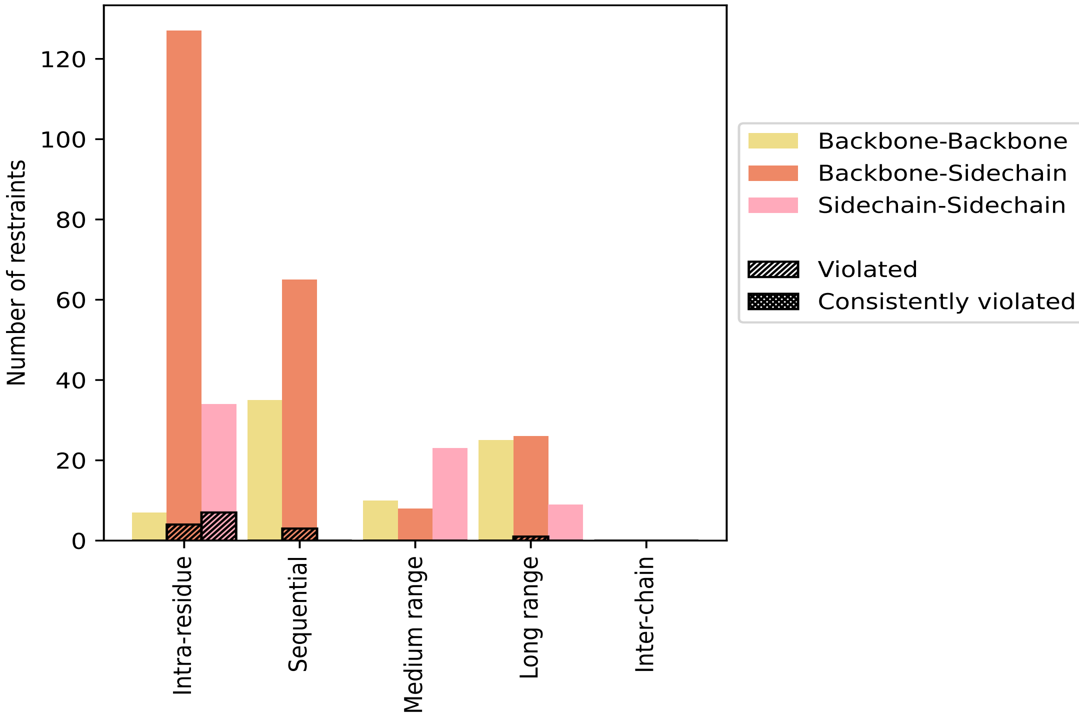
9.1 Summary of distance violations (i)

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)	168	45.5	11	6.5	3.0	0	0.0	0.0
Backbone-Backbone	7	1.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	127	34.4	4	3.1	1.1	0	0.0	0.0
Sidechain-Sidechain	34	9.2	7	20.6	1.9	0	0.0	0.0
Sequential (|i-j|=1)	100	27.1	3	3.0	0.8	0	0.0	0.0
Backbone-Backbone	35	9.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	65	17.6	3	4.6	0.8	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	35	9.5	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	4	1.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	8	2.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	23	6.2	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	46	12.5	1	2.2	0.3	0	0.0	0.0
Backbone-Backbone	11	3.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	26	7.0	1	3.8	0.3	0	0.0	0.0
Sidechain-Sidechain	9	2.4	0	0.0	0.0	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	20	5.4	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	369	100.0	15	4.1	4.1	0	0.0	0.0
Backbone-Backbone	77	20.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	226	61.2	8	3.5	2.2	0	0.0	0.0
Sidechain-Sidechain	66	17.9	7	10.6	1.9	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	0	0	1	0	3	0.22	0.36	0.1	0.19
2	2	0	0	0	0	2	0.23	0.28	0.06	0.23
3	3	0	0	0	0	3	0.21	0.36	0.11	0.16
4	2	0	0	0	0	2	0.24	0.36	0.12	0.24
5	2	1	0	0	0	3	0.23	0.3	0.08	0.27
6	2	0	0	0	0	2	0.22	0.26	0.04	0.22
7	2	0	0	0	0	2	0.28	0.3	0.02	0.28
8	2	1	0	0	0	3	0.22	0.29	0.08	0.26
9	3	1	0	0	0	4	0.19	0.27	0.05	0.18
10	1	1	0	0	0	2	0.24	0.37	0.13	0.24
11	1	0	0	0	0	1	0.35	0.35	0.0	0.35

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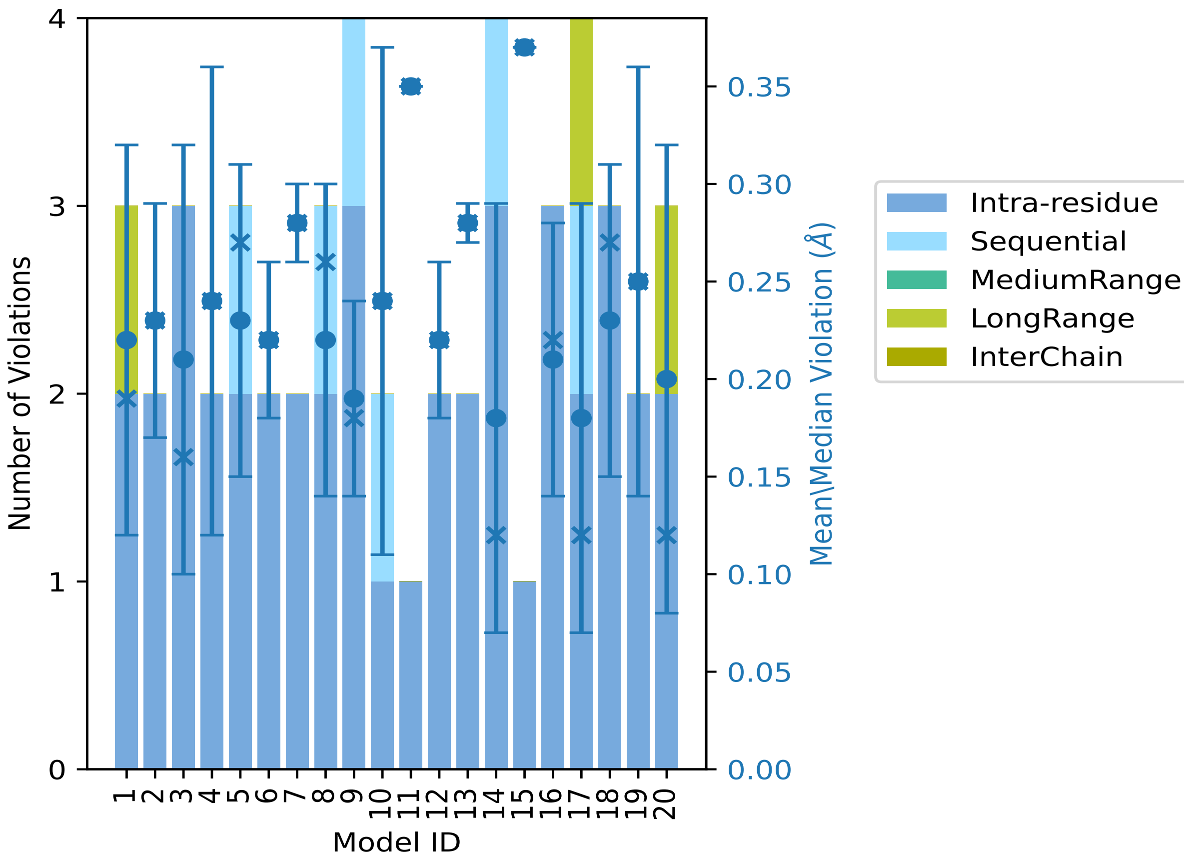
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	2	0	0	0	0	2	0.22	0.25	0.04	0.22
13	2	0	0	0	0	2	0.28	0.29	0.01	0.28
14	3	1	0	0	0	4	0.18	0.36	0.11	0.12
15	1	0	0	0	0	1	0.37	0.37	0.0	0.37
16	3	0	0	0	0	3	0.21	0.29	0.07	0.22
17	2	1	0	1	0	4	0.18	0.36	0.11	0.12
18	3	0	0	0	0	3	0.23	0.3	0.08	0.27
19	2	0	0	0	0	2	0.25	0.36	0.11	0.25
20	2	0	0	1	0	3	0.2	0.36	0.12	0.12

[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

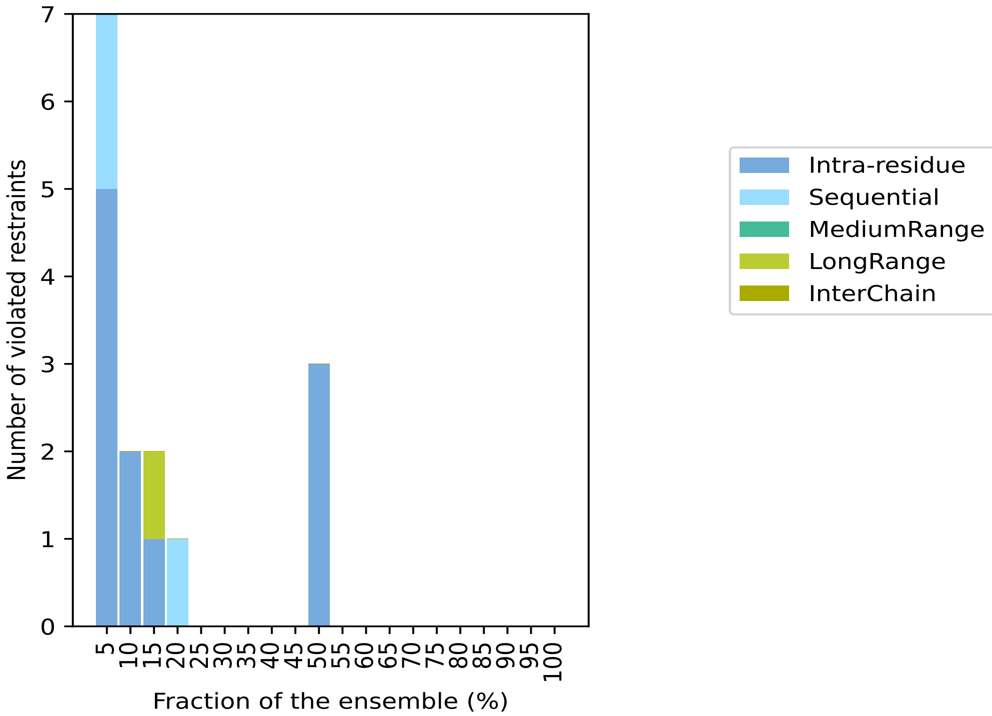
9.3 Distance violation statistics for the ensemble (i)

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, 334(IR:157, SQ:97, MR:35, LR:45, 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]	%
5	2	0	0	0	7	1	5.0
2	0	0	0	0	2	2	10.0
1	0	0	1	0	2	3	15.0
0	1	0	0	0	1	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
3	0	0	0	0	3	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	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

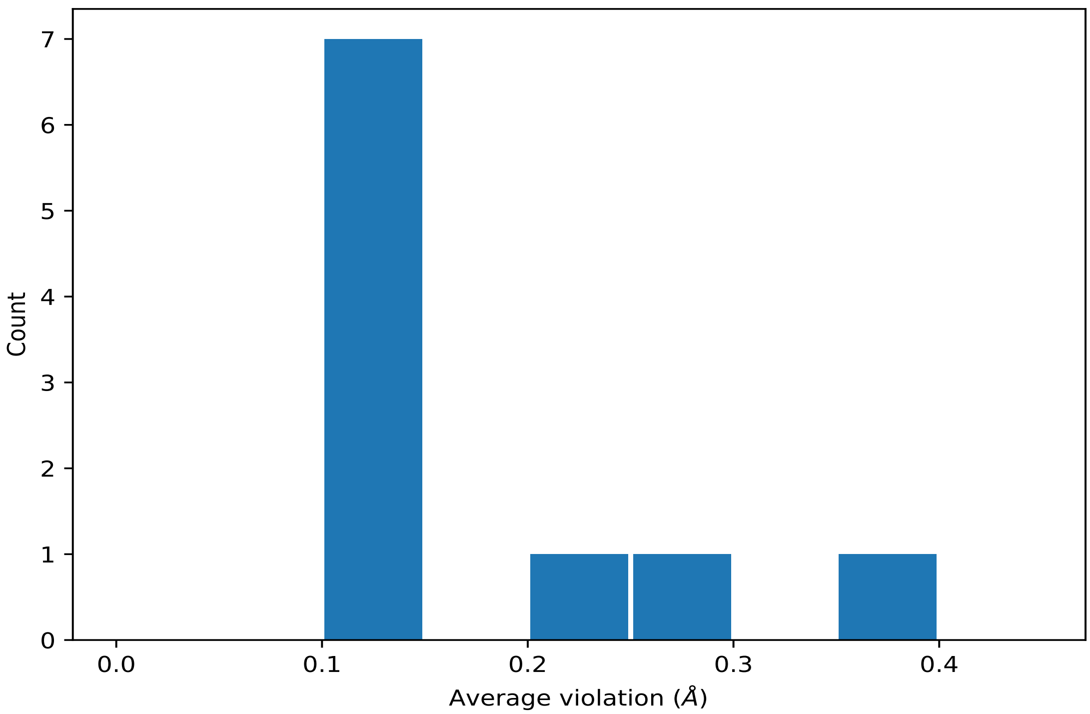
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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.

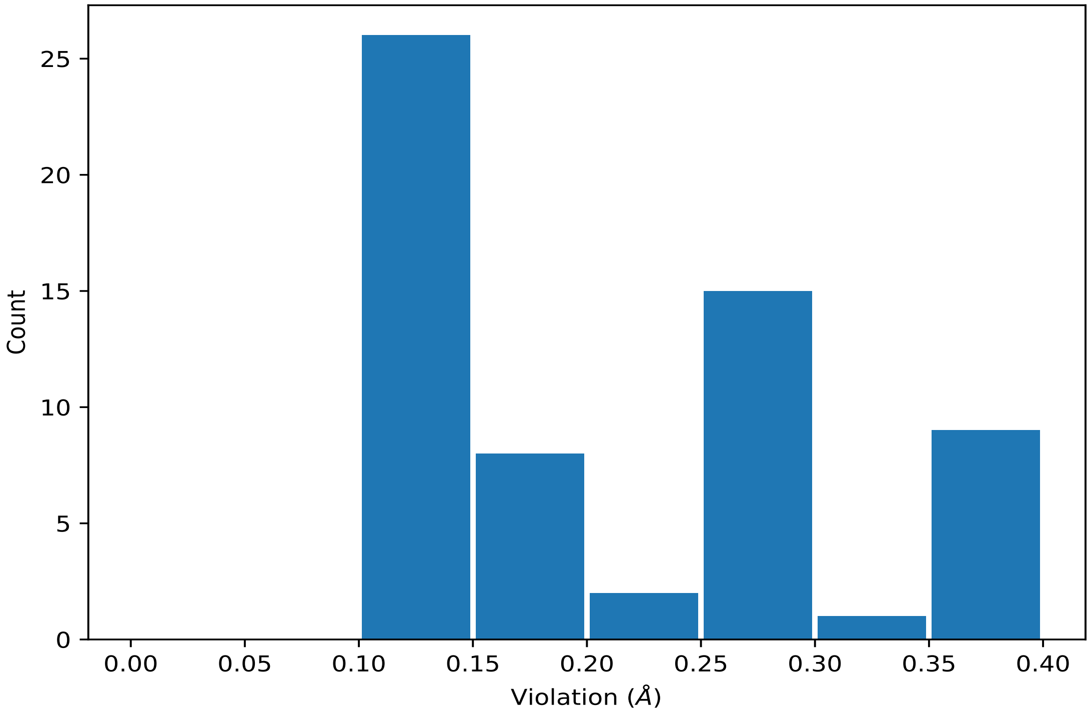
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,181)	1:A:27:ASN:HA	1:A:27:ASN:HB3	10	0.36	0.01	0.36
(2,180)	1:A:27:ASN:HB2	1:A:27:ASN:HD22	10	0.28	0.02	0.29
(2,179)	1:A:27:ASN:HB2	1:A:27:ASN:HD21	10	0.23	0.04	0.24
(2,91)	1:A:12:ARG:HB3	1:A:13:ASN:H	4	0.11	0.0	0.11
(2,140)	1:A:20:LEU:H	1:A:20:LEU:HD11	3	0.12	0.01	0.11
(2,140)	1:A:20:LEU:H	1:A:20:LEU:HD12	3	0.12	0.01	0.11
(2,140)	1:A:20:LEU:H	1:A:20:LEU:HD13	3	0.12	0.01	0.11
(2,296)	1:A:7:TRP:H	1:A:29:CYS:HB3	3	0.11	0.0	0.11
(2,175)	1:A:26:HIS:HB3	1:A:26:HIS:HD2	2	0.12	0.0	0.12
(2,174)	1:A:26:HIS:HB2	1:A:26:HIS:HD2	2	0.11	0.0	0.11

[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)
(2,181)	1:A:27:ASN:HA	1:A:27:ASN:HB3	10	0.37
(2,181)	1:A:27:ASN:HA	1:A:27:ASN:HB3	15	0.37
(2,181)	1:A:27:ASN:HA	1:A:27:ASN:HB3	1	0.36
(2,181)	1:A:27:ASN:HA	1:A:27:ASN:HB3	3	0.36
(2,181)	1:A:27:ASN:HA	1:A:27:ASN:HB3	4	0.36
(2,181)	1:A:27:ASN:HA	1:A:27:ASN:HB3	14	0.36
(2,181)	1:A:27:ASN:HA	1:A:27:ASN:HB3	17	0.36
(2,181)	1:A:27:ASN:HA	1:A:27:ASN:HB3	19	0.36
(2,181)	1:A:27:ASN:HA	1:A:27:ASN:HB3	20	0.36
(2,181)	1:A:27:ASN:HA	1:A:27:ASN:HB3	11	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,180)	1:A:27:ASN:HB2	1:A:27:ASN:HD22	5	0.3
(2,180)	1:A:27:ASN:HB2	1:A:27:ASN:HD22	7	0.3
(2,180)	1:A:27:ASN:HB2	1:A:27:ASN:HD22	18	0.3
(2,180)	1:A:27:ASN:HB2	1:A:27:ASN:HD22	8	0.29
(2,180)	1:A:27:ASN:HB2	1:A:27:ASN:HD22	13	0.29
(2,180)	1:A:27:ASN:HB2	1:A:27:ASN:HD22	16	0.29
(2,180)	1:A:27:ASN:HB2	1:A:27:ASN:HD22	2	0.28
(2,180)	1:A:27:ASN:HB2	1:A:27:ASN:HD22	9	0.27
(2,179)	1:A:27:ASN:HB2	1:A:27:ASN:HD21	5	0.27
(2,179)	1:A:27:ASN:HB2	1:A:27:ASN:HD21	13	0.27
(2,179)	1:A:27:ASN:HB2	1:A:27:ASN:HD21	18	0.27
(2,180)	1:A:27:ASN:HB2	1:A:27:ASN:HD22	6	0.26
(2,179)	1:A:27:ASN:HB2	1:A:27:ASN:HD21	7	0.26
(2,179)	1:A:27:ASN:HB2	1:A:27:ASN:HD21	8	0.26
(2,180)	1:A:27:ASN:HB2	1:A:27:ASN:HD22	12	0.25
(2,179)	1:A:27:ASN:HB2	1:A:27:ASN:HD21	16	0.22
(2,179)	1:A:27:ASN:HB2	1:A:27:ASN:HD21	9	0.2
(2,80)	1:A:10:ASN:HB3	1:A:10:ASN:HD21	1	0.19
(2,179)	1:A:27:ASN:HB2	1:A:27:ASN:HD21	12	0.18
(2,179)	1:A:27:ASN:HB2	1:A:27:ASN:HD21	2	0.17
(2,179)	1:A:27:ASN:HB2	1:A:27:ASN:HD21	6	0.17
(2,90)	1:A:12:ARG:HA	1:A:12:ARG:HD2	3	0.16
(2,90)	1:A:12:ARG:HA	1:A:12:ARG:HD3	3	0.16
(2,329)	1:A:21:LYS:HB2	1:A:22:CYS:H	9	0.16
(2,329)	1:A:21:LYS:HB3	1:A:22:CYS:H	9	0.16
(2,140)	1:A:20:LEU:H	1:A:20:LEU:HD11	19	0.14
(2,140)	1:A:20:LEU:H	1:A:20:LEU:HD12	19	0.14
(2,140)	1:A:20:LEU:H	1:A:20:LEU:HD13	19	0.14
(2,83)	1:A:10:ASN:HB2	1:A:10:ASN:HD22	9	0.13
(2,91)	1:A:12:ARG:HB3	1:A:13:ASN:H	14	0.12
(2,72)	1:A:8:LYS:HD2	1:A:9:CYS:H	5	0.12
(2,72)	1:A:8:LYS:HD3	1:A:9:CYS:H	5	0.12
(2,296)	1:A:7:TRP:H	1:A:29:CYS:HB3	20	0.12
(2,175)	1:A:26:HIS:HB3	1:A:26:HIS:HD2	17	0.12
(2,112)	1:A:15:LYS:HA	1:A:15:LYS:HE2	14	0.12
(2,112)	1:A:15:LYS:HA	1:A:15:LYS:HE3	14	0.12
(2,91)	1:A:12:ARG:HB3	1:A:13:ASN:H	8	0.11
(2,91)	1:A:12:ARG:HB3	1:A:13:ASN:H	10	0.11
(2,91)	1:A:12:ARG:HB3	1:A:13:ASN:H	17	0.11
(2,296)	1:A:7:TRP:H	1:A:29:CYS:HB3	1	0.11
(2,296)	1:A:7:TRP:H	1:A:29:CYS:HB3	17	0.11
(2,189)	1:A:28:TRP:HB2	1:A:28:TRP:HE3	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,175)	1:A:26:HIS:HB3	1:A:26:HIS:HD2	18	0.11
(2,174)	1:A:26:HIS:HB2	1:A:26:HIS:HD2	4	0.11
(2,174)	1:A:26:HIS:HB2	1:A:26:HIS:HD2	16	0.11
(2,140)	1:A:20:LEU:H	1:A:20:LEU:HD11	14	0.11
(2,140)	1:A:20:LEU:H	1:A:20:LEU:HD12	14	0.11
(2,140)	1:A:20:LEU:H	1:A:20:LEU:HD13	14	0.11
(2,140)	1:A:20:LEU:H	1:A:20:LEU:HD11	20	0.11
(2,140)	1:A:20:LEU:H	1:A:20:LEU:HD12	20	0.11
(2,140)	1:A:20:LEU:H	1:A:20:LEU:HD13	20	0.11

10 Dihedral-angle violation analysis (i)

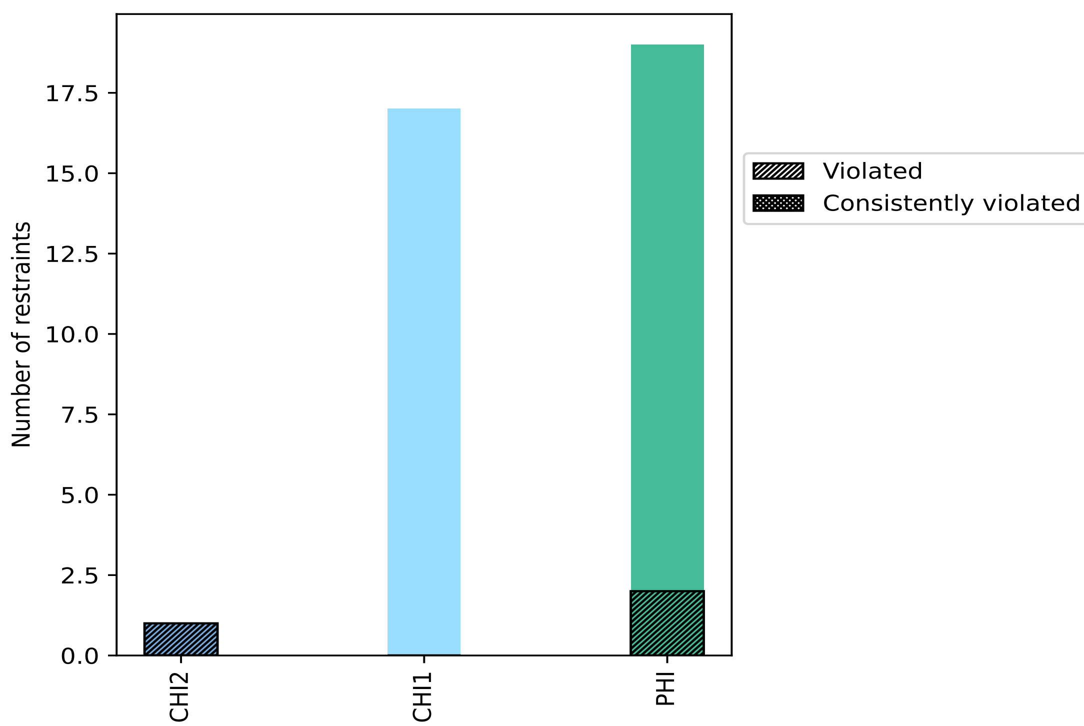
10.1 Summary of dihedral-angle violations (i)

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]
CHI2	1	2.7	1	100.0	2.7	0	0.0	0.0
CHI1	17	45.9	0	0.0	0.0	0	0.0	0.0
PHI	19	51.4	2	10.5	5.4	0	0.0	0.0
Total	37	100.0	3	8.1	8.1	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)



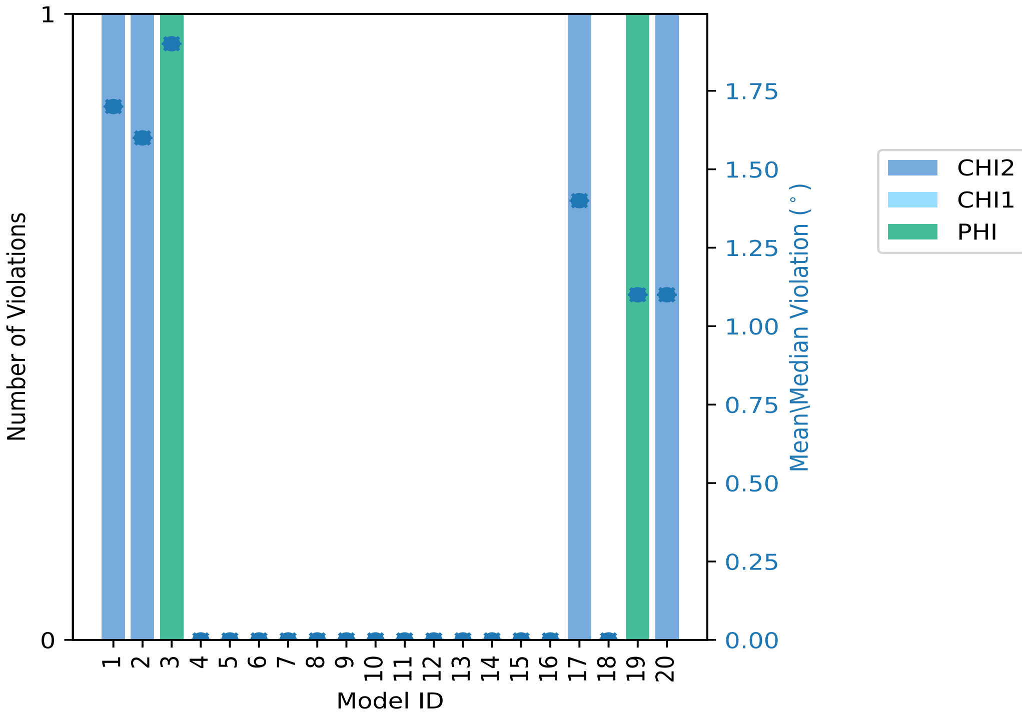
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	CHI2	CHI1	PHI	Total				
1	1	0	0	1	1.7	1.7	0.0	1.7
2	1	0	0	1	1.6	1.6	0.0	1.6
3	0	0	1	1	1.9	1.9	0.0	1.9
4	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0	0.0	0.0	0.0	0.0
17	1	0	0	1	1.4	1.4	0.0	1.4
18	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	1	1	1.1	1.1	0.0	1.1
20	1	0	0	1	1.1	1.1	0.0	1.1

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	
CHI2	CHI1	PHI	Total	Count[1]	%
0	0	2	2	1	5.0
0	0	0	0	2	10.0
0	0	0	0	3	15.0
1	0	0	1	4	20.0
0	0	0	0	5	25.0
0	0	0	0	6	30.0
0	0	0	0	7	35.0
0	0	0	0	8	40.0
0	0	0	0	9	45.0
0	0	0	0	10	50.0
0	0	0	0	11	55.0

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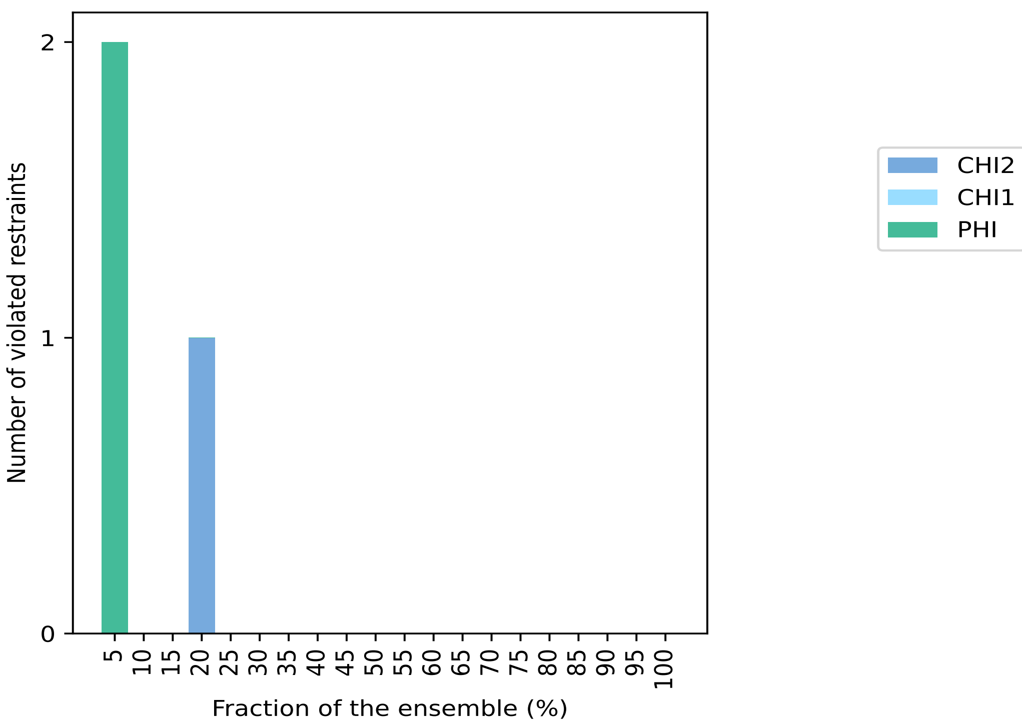
Number of violated restraints				Fraction of the ensemble	
CHI2	CHI1	PHI	Total	Count[1]	%
0	0	0	0	12	60.0
0	0	0	0	13	65.0
0	0	0	0	14	70.0
0	0	0	0	15	75.0
0	0	0	0	16	80.0
0	0	0	0	17	85.0
0	0	0	0	18	90.0
0	0	0	0	19	95.0
0	0	0	0	20	100.0

[1] Number of models with violations

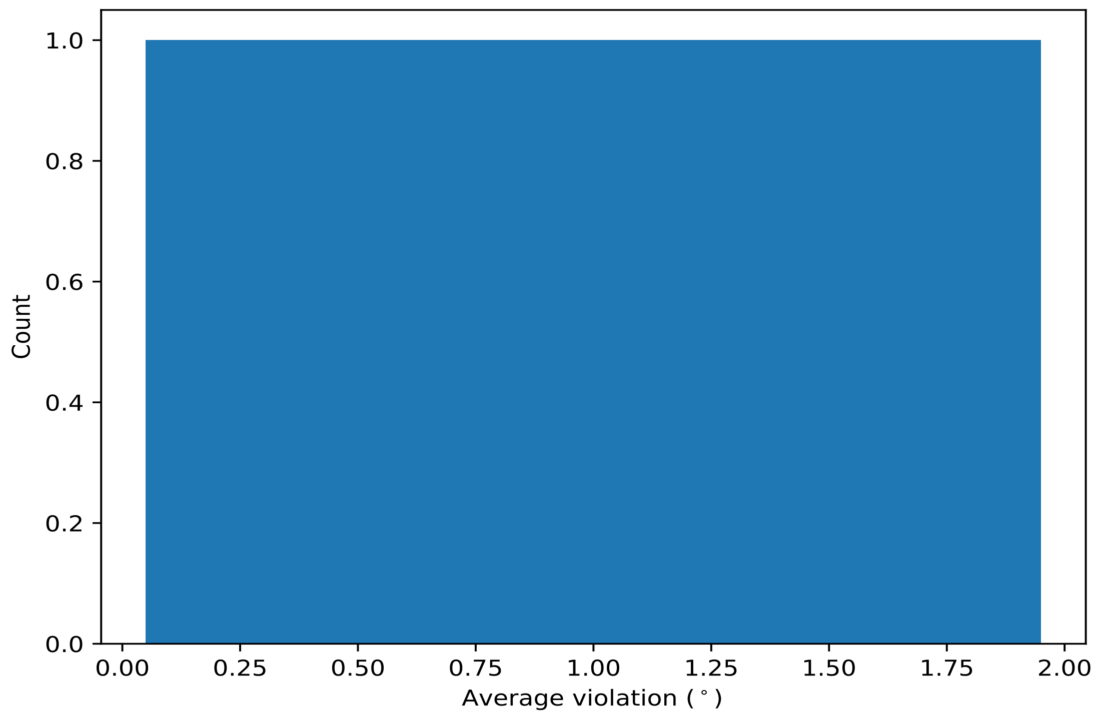
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)



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 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.

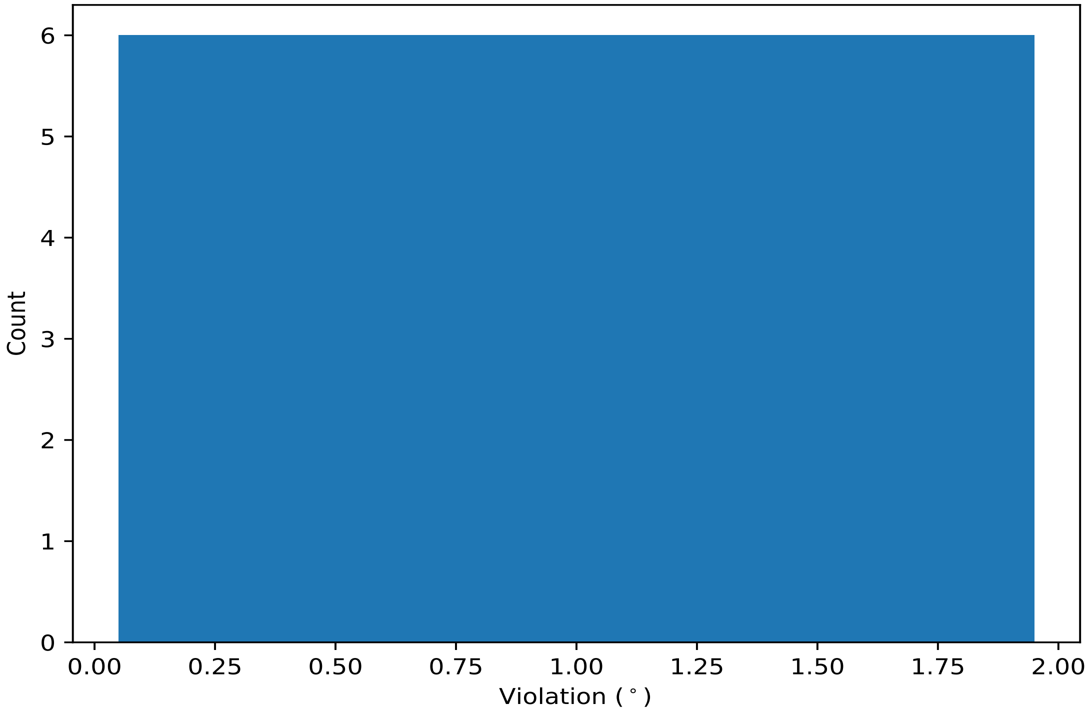
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,37)	1:A:28:TRP:CA	1:A:28:TRP:CB	1:A:28:TRP:CG	1:A:28:TRP:CD1	4	1.45	0.23	1.5

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



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

The following table 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 (°)
(1,1)	1:A:1:ASP:C	1:A:2:CYS:N	1:A:2:CYS:CA	1:A:2:CYS:C	3	1.9
(1,37)	1:A:28:TRP:CA	1:A:28:TRP:CB	1:A:28:TRP:CG	1:A:28:TRP:CD1	1	1.7
(1,37)	1:A:28:TRP:CA	1:A:28:TRP:CB	1:A:28:TRP:CG	1:A:28:TRP:CD1	2	1.6
(1,37)	1:A:28:TRP:CA	1:A:28:TRP:CB	1:A:28:TRP:CG	1:A:28:TRP:CD1	17	1.4
(1,37)	1:A:28:TRP:CA	1:A:28:TRP:CB	1:A:28:TRP:CG	1:A:28:TRP:CD1	20	1.1
(1,14)	1:A:20:LEU:C	1:A:21:LYS:N	1:A:21:LYS:CA	1:A:21:LYS:C	19	1.1