



wwPDB NMR Structure Validation Summary Report ⓘ

Jun 6, 2023 – 08:58 pm BST

PDB ID : 6YQ5
EMDB ID : EMD-10792
BMRB ID : 27468
Title : Hybrid structure of the SPP1 tail tube by solid-state NMR and cryo EM -
NMR Ensemble
Authors : Zinke, M.; Sachowsky, K.A.A.; Zinn-Justin, S.; Ravelli, R.; Schroder, G.F.;
Habeck, M.; Lange, A.
Deposited on : 2020-04-16

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : **NOT EXECUTED**
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **NOT EXECUTED**
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

The following experimental techniques were used to determine the structure:

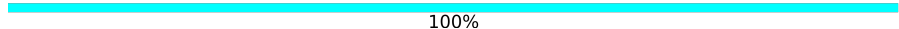



ELECTRON MICROSCOPY, SOLID-STATE NMR

The reported resolution of this entry is 4.00 Å.

The overall completeness of chemical shifts assignment was not calculated.

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

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	172	 100%
1	B	172	 100%
1	C	172	 100%
1	D	172	 100%
1	E	172	 100%
1	F	172	 100%
1	G	172	 100%
1	H	172	 100%
1	I	172	 100%
1	J	172	 100%
1	K	172	 100%
1	L	172	 100%

2 Ensemble composition and analysis

This entry contains 10 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores.

Cyrange was unable to find well-defined residues.

Error message: Cyrange did not run

NmrClust was unable to cluster the ensemble.

Error message: NmrClust did not run

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 30672 atoms, of which 14916 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tail tube protein gp17.1*.

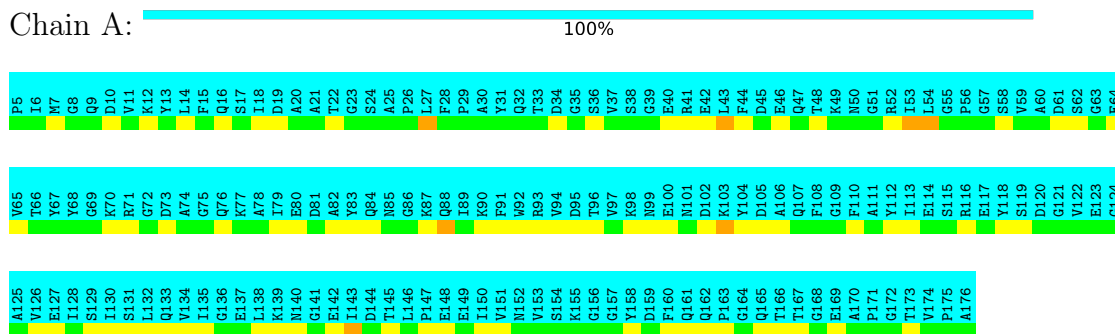
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	172	2556	821	1243	216	275	1	0	
1	B	172	2556	821	1243	216	275	1	0	
1	C	172	2556	821	1243	216	275	1	0	
1	D	172	2556	821	1243	216	275	1	0	
1	E	172	2556	821	1243	216	275	1	0	
1	F	172	2556	821	1243	216	275	1	0	
1	G	172	2556	821	1243	216	275	1	0	
1	H	172	2556	821	1243	216	275	1	0	
1	I	172	2556	821	1243	216	275	1	0	
1	J	172	2556	821	1243	216	275	1	0	
1	K	172	2556	821	1243	216	275	1	0	
1	L	172	2556	821	1243	216	275	1	0	

4 Residue-property plots [i](#)

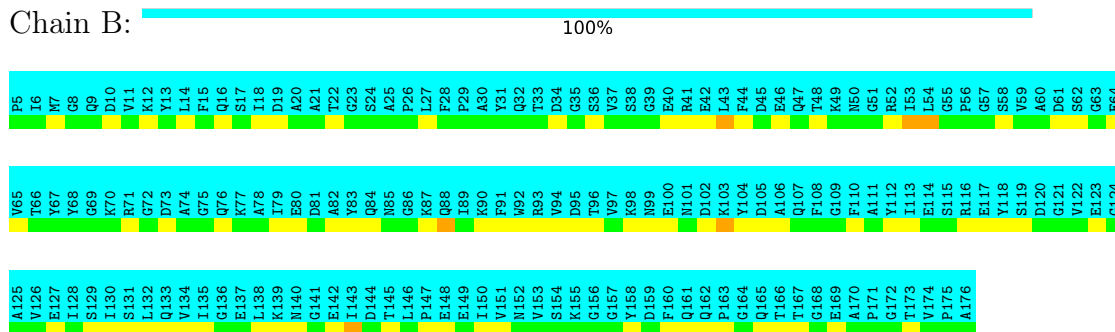
4.1 Average score per residue in the NMR ensemble

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.

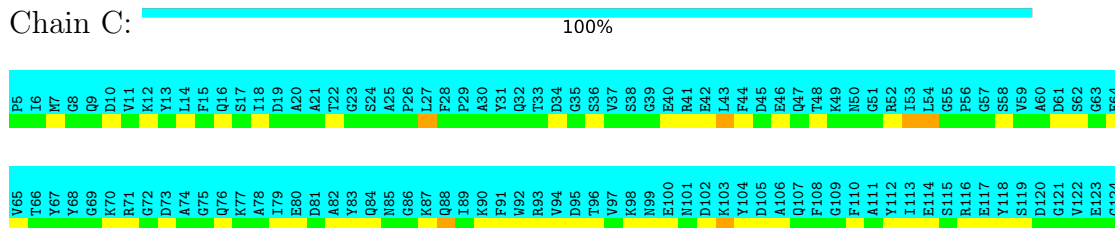
- Molecule 1: Tail tube protein gp17.1*

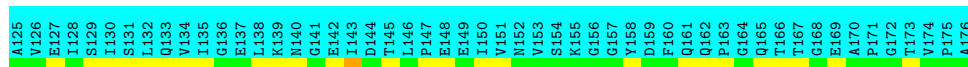


- Molecule 1: Tail tube protein gp17.1*



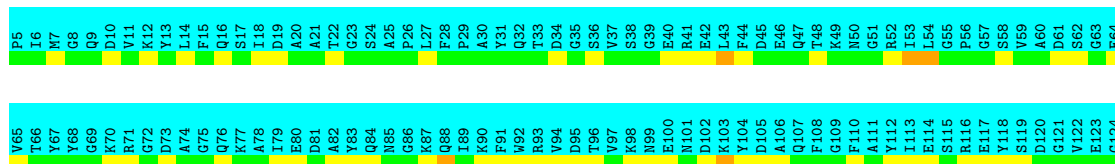
- Molecule 1: Tail tube protein gp17.1*





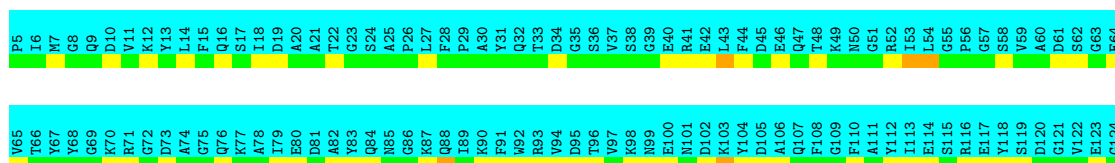
- Molecule 1: Tail tube protein gp17.1*

Chain D:



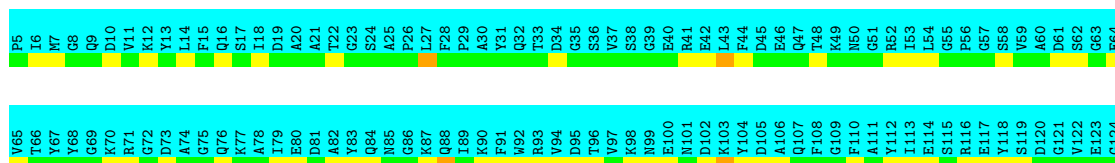
- Molecule 1: Tail tube protein gp17.1*

Chain E:



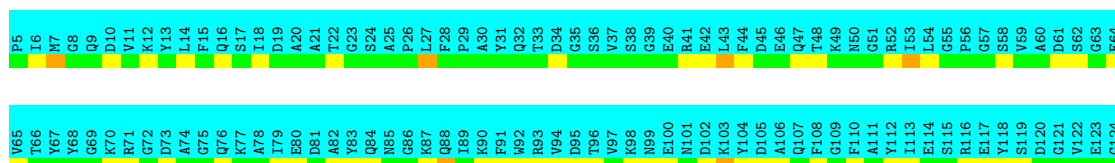
- Molecule 1: Tail tube protein gp17.1*

Chain F:



- Molecule 1: Tail tube protein gp17.1*

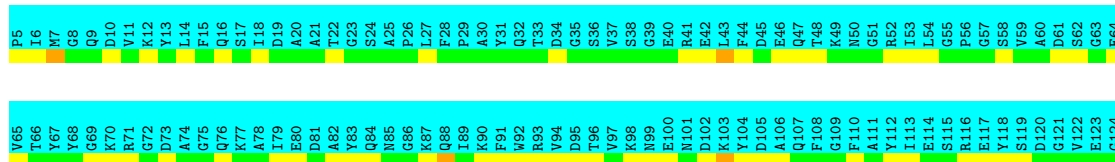
Chain G:





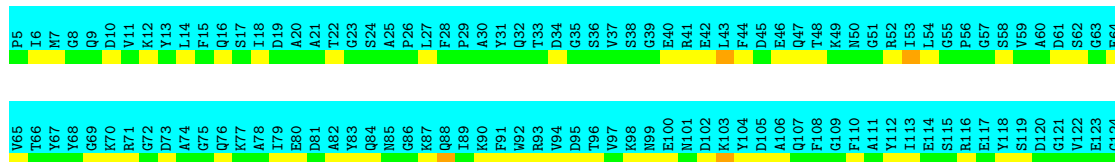
• Molecule 1: Tail tube protein gp17.1*

Chain H: 100%



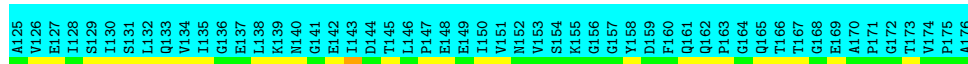
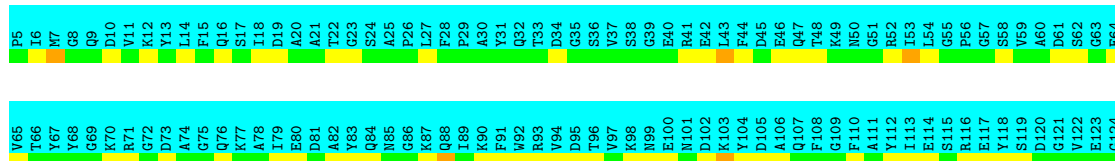
• Molecule 1: Tail tube protein gp17.1*

Chain I: 100%



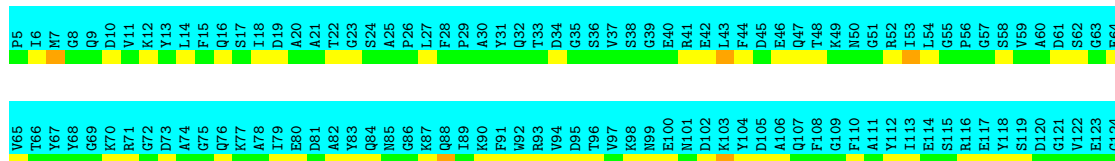
• Molecule 1: Tail tube protein gp17.1*

Chain J: 100%



• Molecule 1: Tail tube protein gp17.1*

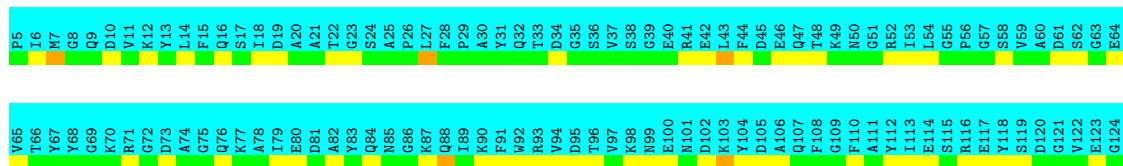
Chain K: 100%





• Molecule 1: Tail tube protein gp17.1*

Chain L:  100%

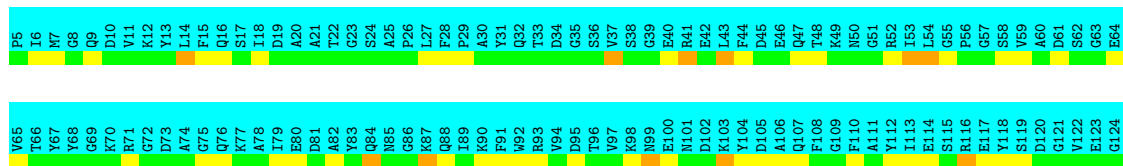


4.2 Residue scores for the representative (author defined) model from the NMR ensemble

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

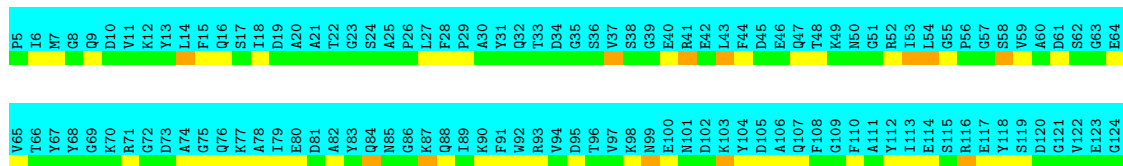
• Molecule 1: Tail tube protein gp17.1*

Chain A:  100%



• Molecule 1: Tail tube protein gp17.1*

Chain B:  100%



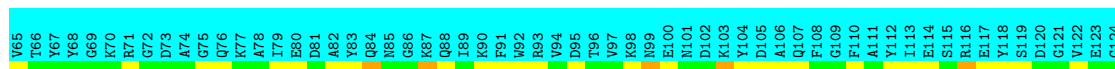
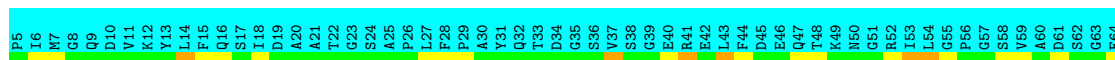
• Molecule 1: Tail tube protein gp17.1*

Chain C:  100%



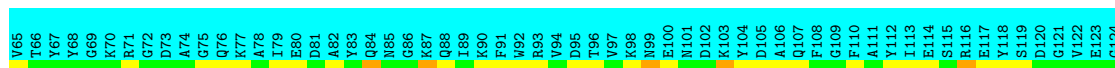
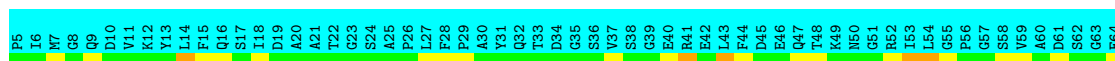
• Molecule 1: Tail tube protein gp17.1*

Chain D: 100%



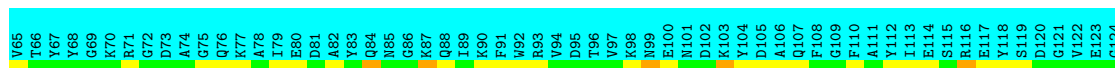
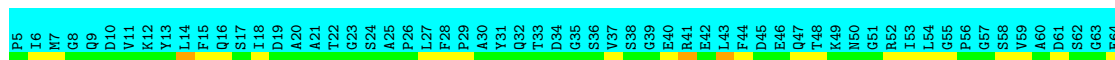
• Molecule 1: Tail tube protein gp17.1*

Chain E: 100%



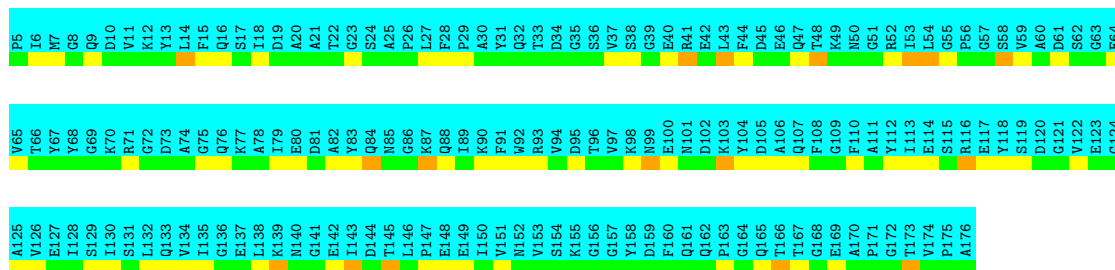
• Molecule 1: Tail tube protein gp17.1*

Chain F: 100%



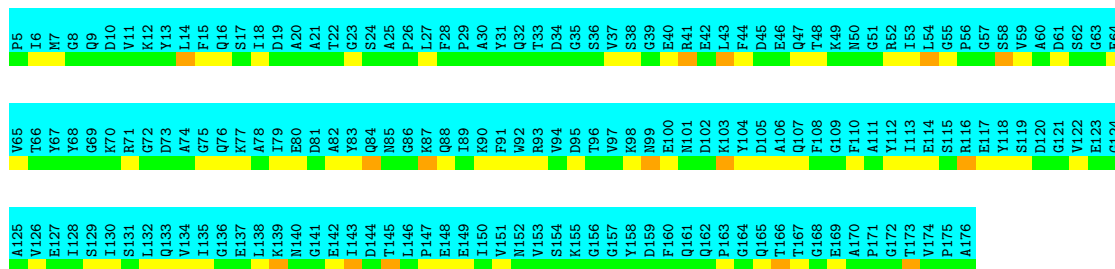
• Molecule 1: Tail tube protein gp17.1*

Chain G: 100%



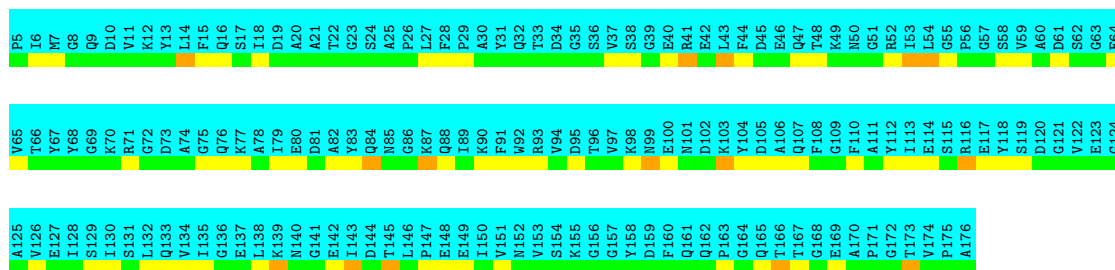
• Molecule 1: Tail tube protein gp17.1*

Chain H: 100%



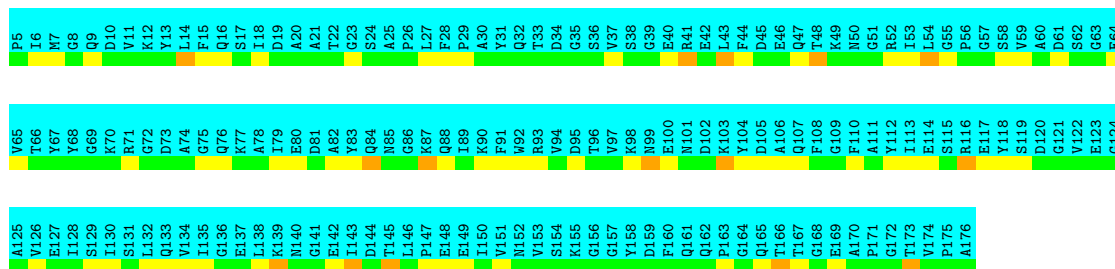
• Molecule 1: Tail tube protein gp17.1*

Chain I: 100%



• Molecule 1: Tail tube protein gp17.1*

Chain J: 100%



• Molecule 1: Tail tube protein gp17.1*

Chain K: 100%



● Molecule 1: Tail tube protein gp17.1*

Chain L:  100%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *na*.

Of the 500 calculated structures, 10 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
Inferential Structure Determination (ISD)	structure calculation	

No chemical shift data was provided. Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality

6.1 Standard geometry

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

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	0	0	0	0±0
1	B	0	0	0	0±0
1	C	0	0	0	0±0
1	D	0	0	0	0±0
1	E	0	0	0	0±0
1	F	0	0	0	0±0
1	G	0	0	0	0±0
1	H	0	0	0	0±0
1	I	0	0	0	0±0
1	J	0	0	0	0±0
1	K	0	0	0	0±0
1	L	0	0	0	0±0
All	All	0	0	0	-

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 -.

There are no clashes.

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	0	-	-	-	-
1	B	0	-	-	-	-
1	C	0	-	-	-	-
1	D	0	-	-	-	-
1	E	0	-	-	-	-
1	F	0	-	-	-	-
1	G	0	-	-	-	-
1	H	0	-	-	-	-
1	I	0	-	-	-	-
1	J	0	-	-	-	-
1	K	0	-	-	-	-
1	L	0	-	-	-	-
All	All	0	-	-	-	-

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	0	-	-	-
1	B	0	-	-	-
1	C	0	-	-	-
1	D	0	-	-	-
1	E	0	-	-	-
1	F	0	-	-	-
1	G	0	-	-	-
1	H	0	-	-	-
1	I	0	-	-	-
1	J	0	-	-	-

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	0	-	-	-
1	L	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

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.

CHEMICAL-SHIFTS INFOmissingINFO

7 NMR restraints analysis [i](#)

7.1 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	1384
Intra-residue ($ i-j =0$)	24
Sequential ($ i-j =1$)	188
Medium range ($ i-j >1$ and $ i-j <5$)	144
Long range ($ i-j \geq 5$)	920
Inter-chain	0
Hydrogen bond restraints	108
Disulfide bond restraints	0
Total dihedral-angle restraints	2880
Number of unmapped restraints	0
Number of restraints per residue	2.1
Number of long range restraints per residue ¹	0.5

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

7.2 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.

7.2.1 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)	27.8	0.2
0.2-0.5 (Medium)	39.4	0.5
>0.5 (Large)	675.1	70.55

7.2.2 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)	633.0	10.0
10.0-20.0 (Medium)	392.9	20.0
>20.0 (Large)	753.6	174.9

8 Distance violation analysis

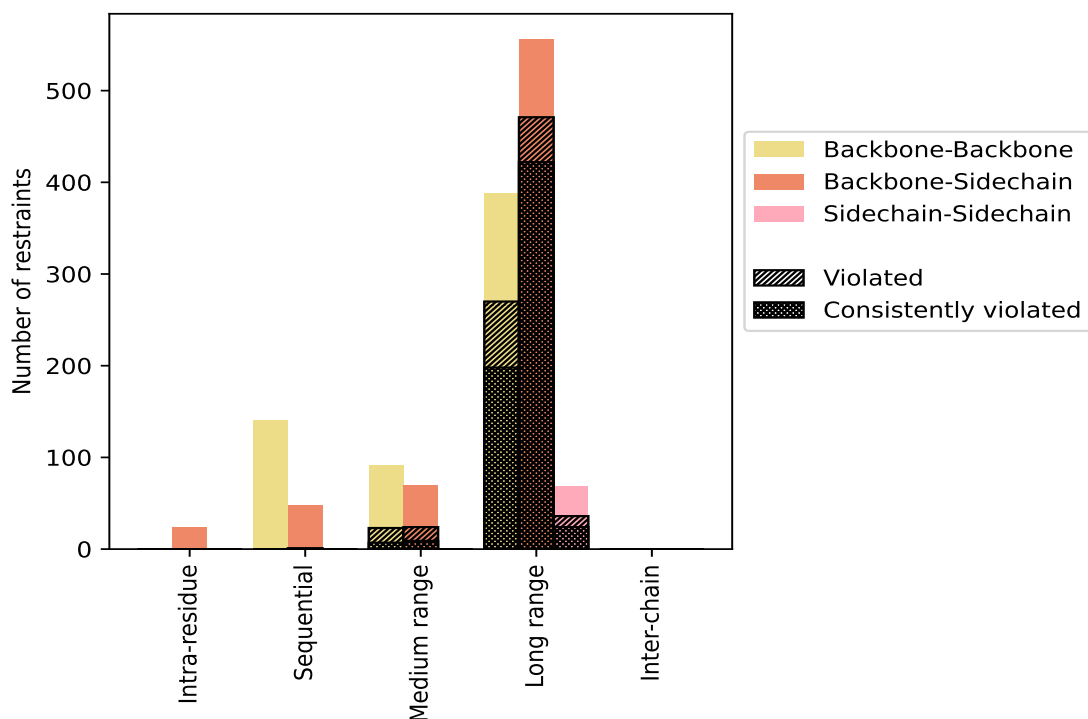
8.1 Summary of distance violations

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 ($i-j =0$)	24	1.7	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	24	1.7	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
Sequential ($i-j =1$)	188	13.6	1	0.5	0.1	0	0.0	0.0
Backbone-Backbone	140	10.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	48	3.5	1	2.1	0.1	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	144	10.4	39	27.1	2.8	15	10.4	1.1
Backbone-Backbone	75	5.4	15	20.0	1.1	6	8.0	0.4
Backbone-Sidechain	69	5.0	24	34.8	1.7	9	13.0	0.7
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	920	66.5	714	77.6	51.6	630	68.5	45.5
Backbone-Backbone	296	21.4	207	69.9	15.0	184	62.2	13.3
Backbone-Sidechain	556	40.2	471	84.7	34.0	422	75.9	30.5
Sidechain-Sidechain	68	4.9	36	52.9	2.6	24	35.3	1.7
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	108	7.8	71	65.7	5.1	15	13.9	1.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1384	100.0	825	59.6	59.6	660	47.7	47.7
Backbone-Backbone	619	44.7	293	47.3	21.2	205	33.1	14.8
Backbone-Sidechain	697	50.4	496	71.2	35.8	431	61.8	31.1
Sidechain-Sidechain	68	4.9	36	52.9	2.6	24	35.3	1.7

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

8.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



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

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

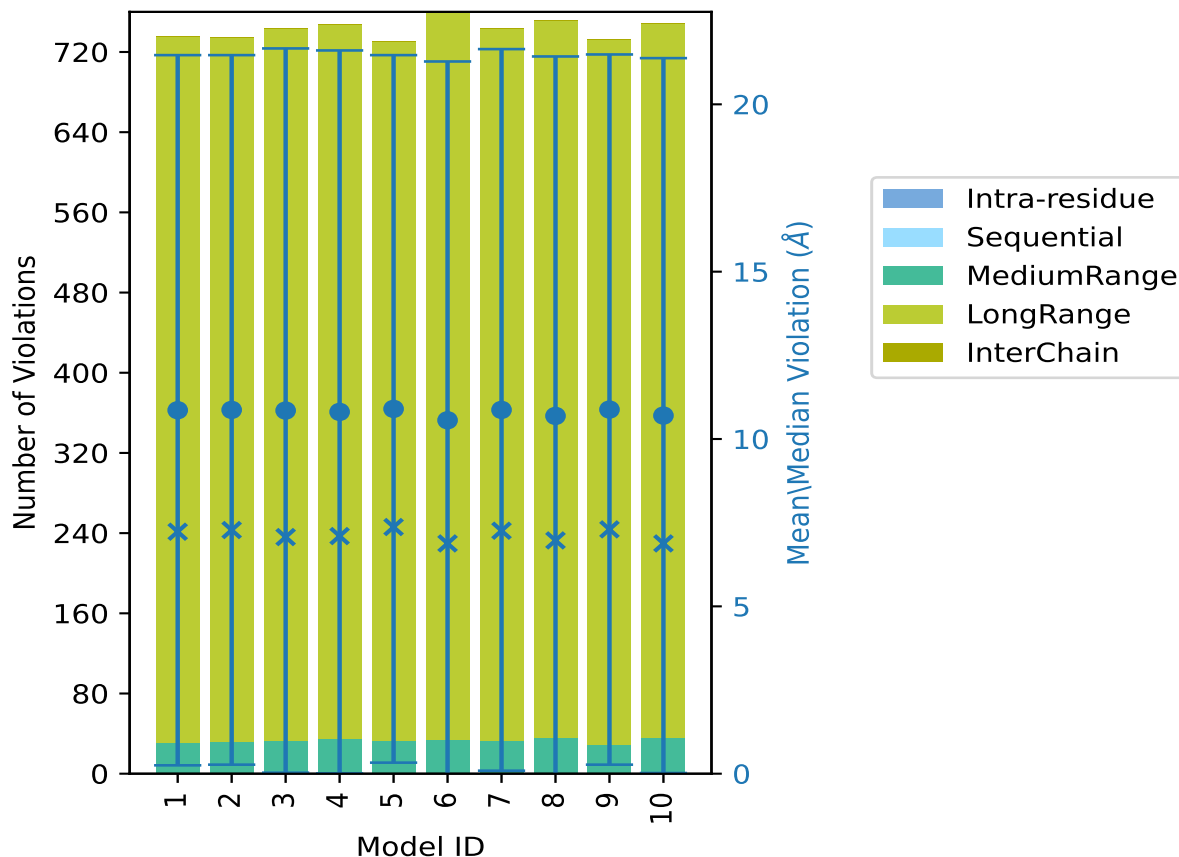
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

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	0	1	30	704	0	735	10.86	66.1	10.61	7.23
2	0	1	31	702	0	734	10.87	66.32	10.6	7.28
3	0	1	32	710	0	743	10.85	69.31	10.82	7.07
4	0	1	34	712	0	747	10.81	69.18	10.8	7.1
5	0	1	32	697	0	730	10.9	66.09	10.57	7.37
6	0	1	33	726	0	760	10.56	70.48	10.72	6.88
7	0	1	32	710	0	743	10.87	69.09	10.78	7.26
8	0	1	35	715	0	751	10.69	70.55	10.74	6.97
9	0	0	29	703	0	732	10.88	66.23	10.61	7.3
10	0	1	35	712	0	748	10.7	70.33	10.68	6.88

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

⁵Inter-chain restraints, ⁶Standard deviation

8.2.1 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

8.3 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, 522(IR:24, SQ:187, MR:105, LR:206, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	1	7	0	8	1	10.0
0	0	3	4	0	7	2	20.0
0	0	4	15	0	19	3	30.0
0	0	1	13	0	14	4	40.0

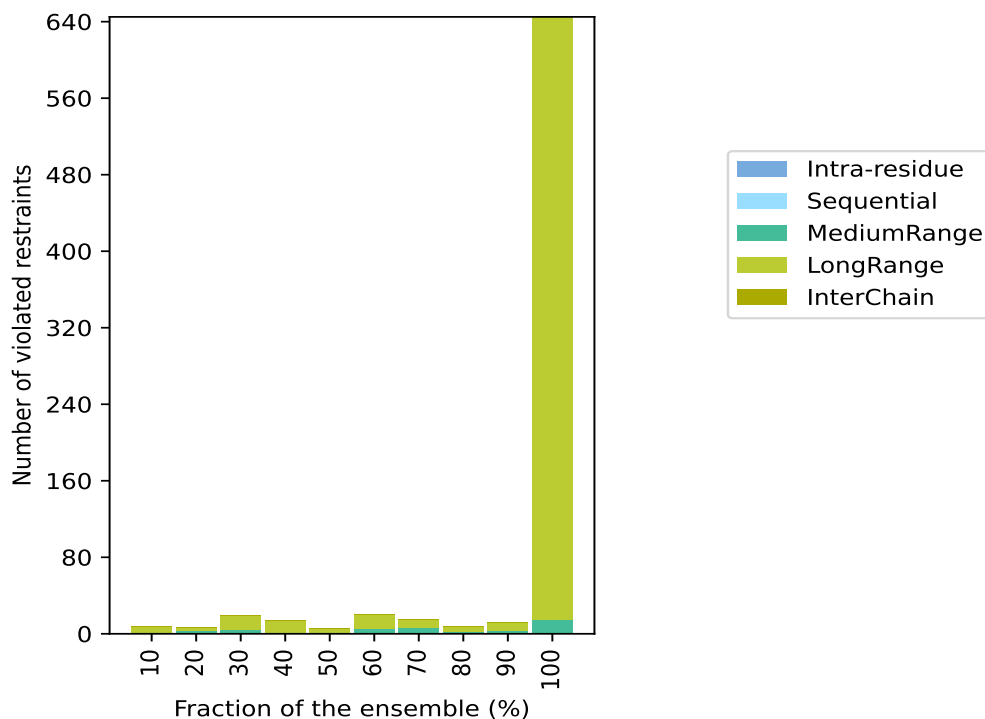
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	6	0	6	5	50.0
0	0	5	15	0	20	6	60.0
0	0	6	9	0	15	7	70.0
0	0	2	6	0	8	8	80.0
0	1	2	9	0	12	9	90.0
0	0	15	630	0	645	10	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶ Number of models with violations

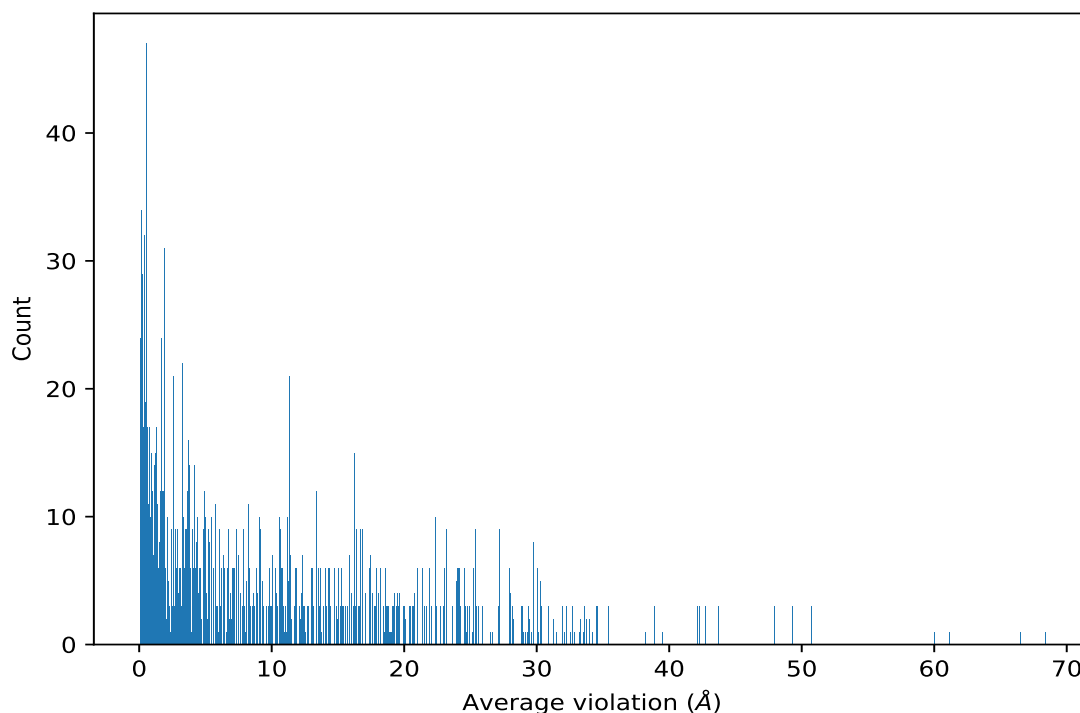
8.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

8.4.1 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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,114)	1:A:161:GLN:H	1:A:48:THR:H	10	68.37	1.85	69.14
(2,116)	1:A:161:GLN:H	1:A:47:GLN:H	10	66.48	1.26	66.8
(2,429)	1:A:160:PHE:H	1:A:52:ARG:H	10	61.13	0.5	60.88
(2,112)	1:A:161:GLN:H	1:A:53:ILE:H	10	60.0	0.13	60.02
(2,1179)	1:A:165:GLN:H	1:A:53:ILE:HG21	10	50.7	0.87	50.26
(2,1179)	1:A:165:GLN:H	1:A:53:ILE:HG22	10	50.7	0.87	50.26
(2,1179)	1:A:165:GLN:H	1:A:53:ILE:HG23	10	50.7	0.87	50.26
(2,1126)	1:A:46:GLU:H	1:A:173:THR:HG21	10	49.28	0.95	49.18
(2,1126)	1:A:46:GLU:H	1:A:173:THR:HG22	10	49.28	0.95	49.18
(2,1126)	1:A:46:GLU:H	1:A:173:THR:HG23	10	49.28	0.95	49.18
(2,612)	1:A:161:GLN:H	1:A:53:ILE:HD11	10	47.96	1.1	48.52
(2,612)	1:A:161:GLN:H	1:A:53:ILE:HD12	10	47.96	1.1	48.52
(2,612)	1:A:161:GLN:H	1:A:53:ILE:HD13	10	47.96	1.1	48.52
(2,766)	1:A:169:GLU:H	1:A:53:ILE:HD11	10	43.71	0.79	44.02
(2,766)	1:A:169:GLU:H	1:A:53:ILE:HD12	10	43.71	0.79	44.02
(2,766)	1:A:169:GLU:H	1:A:53:ILE:HD13	10	43.71	0.79	44.02

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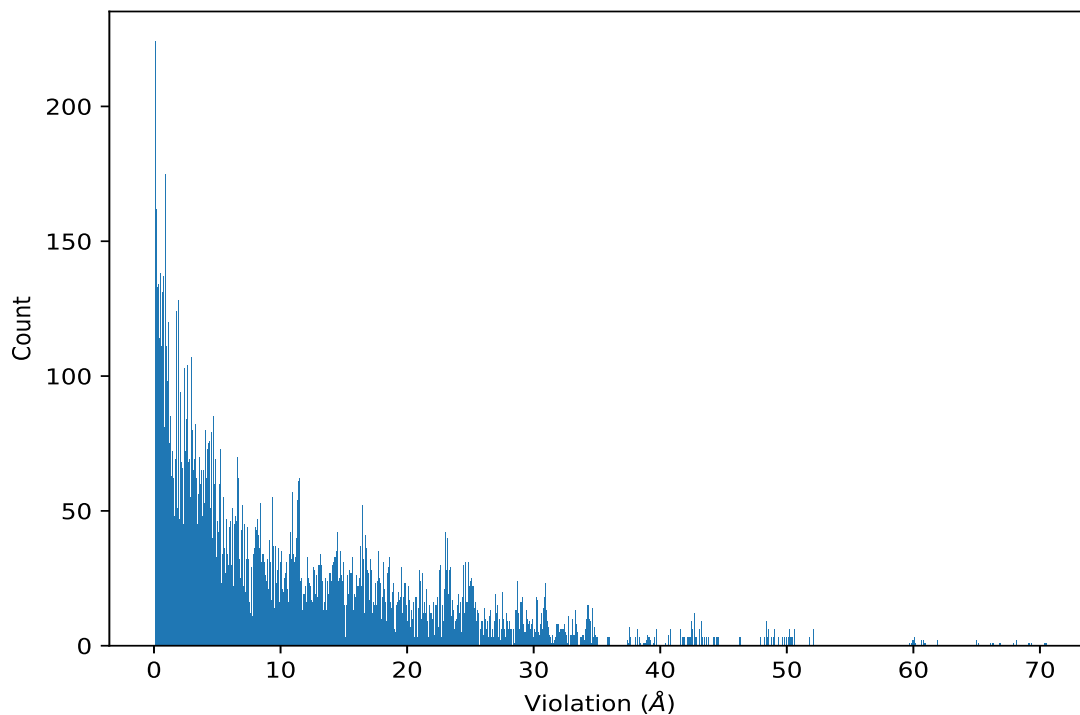
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,774)	1:A:172:GLY:H	1:A:53:ILE:HD11	10	42.73	0.47	42.54
(2,774)	1:A:172:GLY:H	1:A:53:ILE:HD12	10	42.73	0.47	42.54
(2,774)	1:A:172:GLY:H	1:A:53:ILE:HD13	10	42.73	0.47	42.54
(2,1146)	1:A:170:ALA:H	1:A:53:ILE:HG21	10	42.27	0.53	42.3

¹Number of violated models, ²Standard deviation

8.5 All violated distance restraints [i](#)

8.5.1 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.



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,114)	1:A:161:GLN:H	1:A:48:THR:H	8	70.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,114)	1:A:161:GLN:H	1:A:48:THR:H	6	70.48
(2,114)	1:A:161:GLN:H	1:A:48:THR:H	10	70.33
(2,114)	1:A:161:GLN:H	1:A:48:THR:H	3	69.31
(2,114)	1:A:161:GLN:H	1:A:48:THR:H	4	69.18
(2,114)	1:A:161:GLN:H	1:A:48:THR:H	7	69.09
(2,116)	1:A:161:GLN:H	1:A:47:GLN:H	8	68.13
(2,116)	1:A:161:GLN:H	1:A:47:GLN:H	6	68.12
(2,116)	1:A:161:GLN:H	1:A:47:GLN:H	10	67.86
(2,116)	1:A:161:GLN:H	1:A:47:GLN:H	3	66.88

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

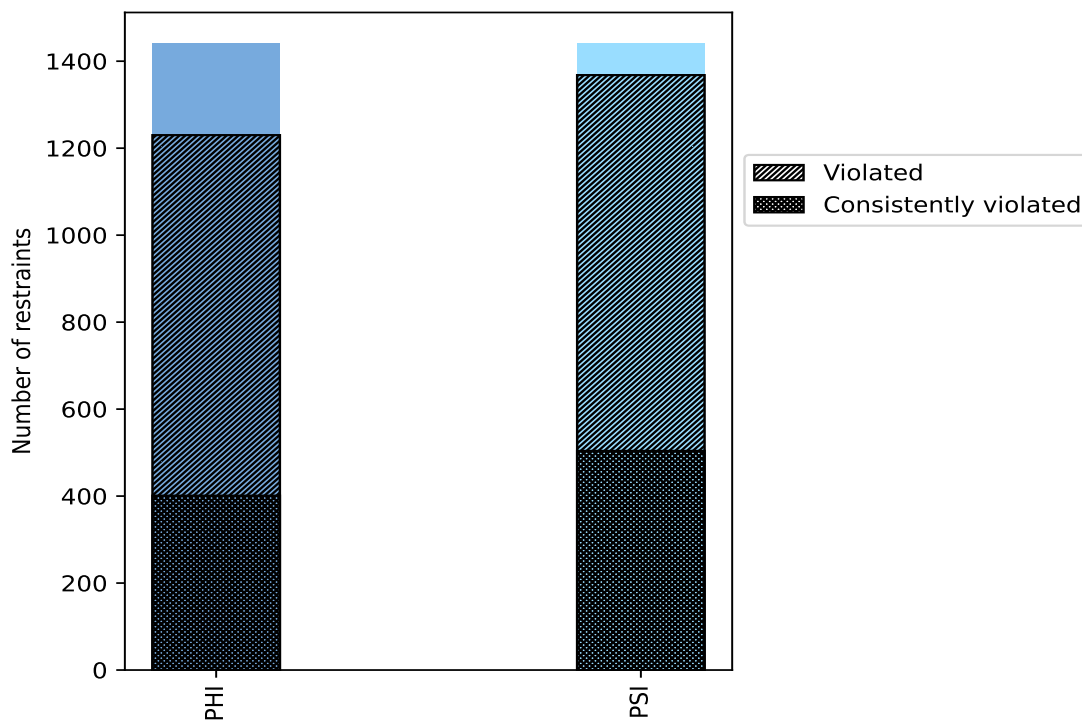
9.1 Summary of dihedral-angle violations [i](#)

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	1440	50.0	1230	85.4	42.7	401	27.8	13.9
PSI	1440	50.0	1368	95.0	47.5	504	35.0	17.5
Total	2880	100.0	2598	90.2	90.2	905	31.4	31.4

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

9.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



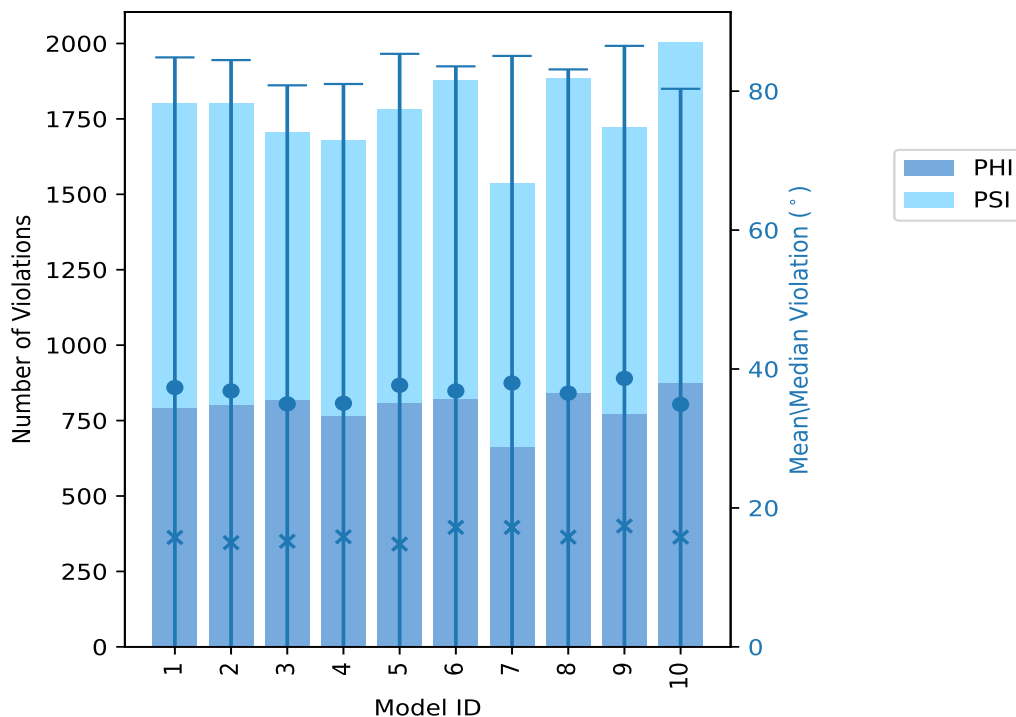
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

9.2 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	792	1008	1800	37.33	170.8	47.53	15.75
2	804	999	1803	36.84	172.7	47.63	15.0
3	817	888	1705	34.98	169.4	45.86	15.2
4	768	912	1680	35.07	168.5	45.96	15.85
5	810	972	1782	37.66	174.9	47.71	14.8
6	821	1056	1877	36.84	174.6	46.73	17.2
7	664	875	1539	37.98	169.0	47.09	17.2
8	840	1044	1884	36.53	173.8	46.6	15.8
9	773	948	1721	38.65	174.9	47.87	17.4
10	876	1128	2004	34.91	167.7	45.43	15.8

9.2.1 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

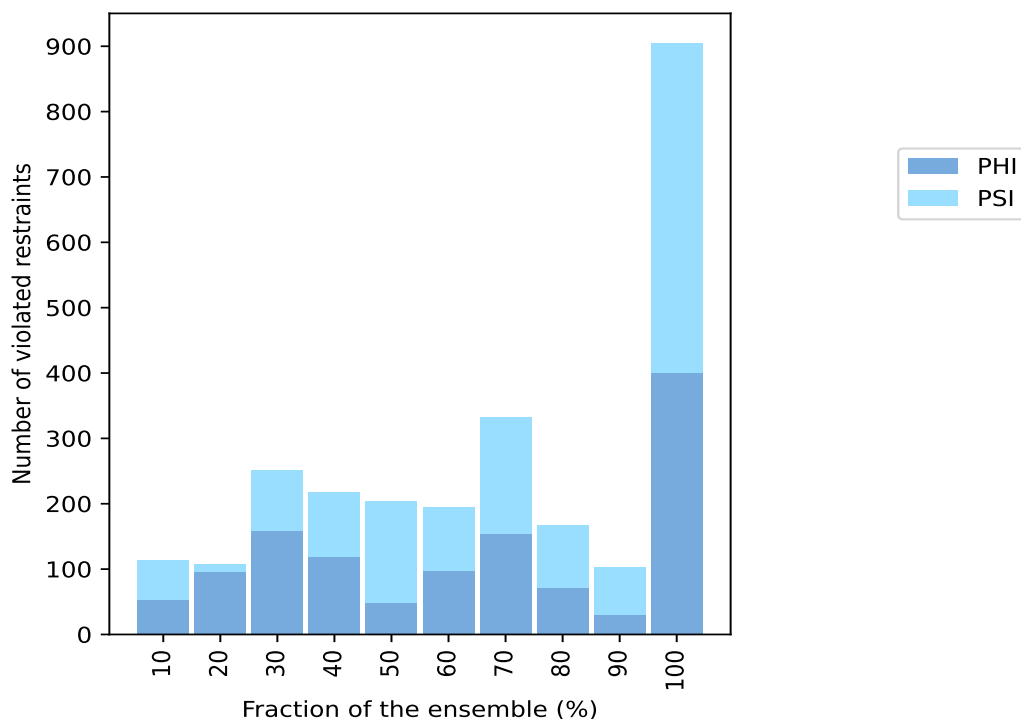
9.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
54	60	114	1	10.0
95	12	107	2	20.0
158	93	251	3	30.0
119	99	218	4	40.0
48	156	204	5	50.0
98	97	195	6	60.0
154	179	333	7	70.0
72	96	168	8	80.0
31	72	103	9	90.0
401	504	905	10	100.0

¹ Number of models with violations

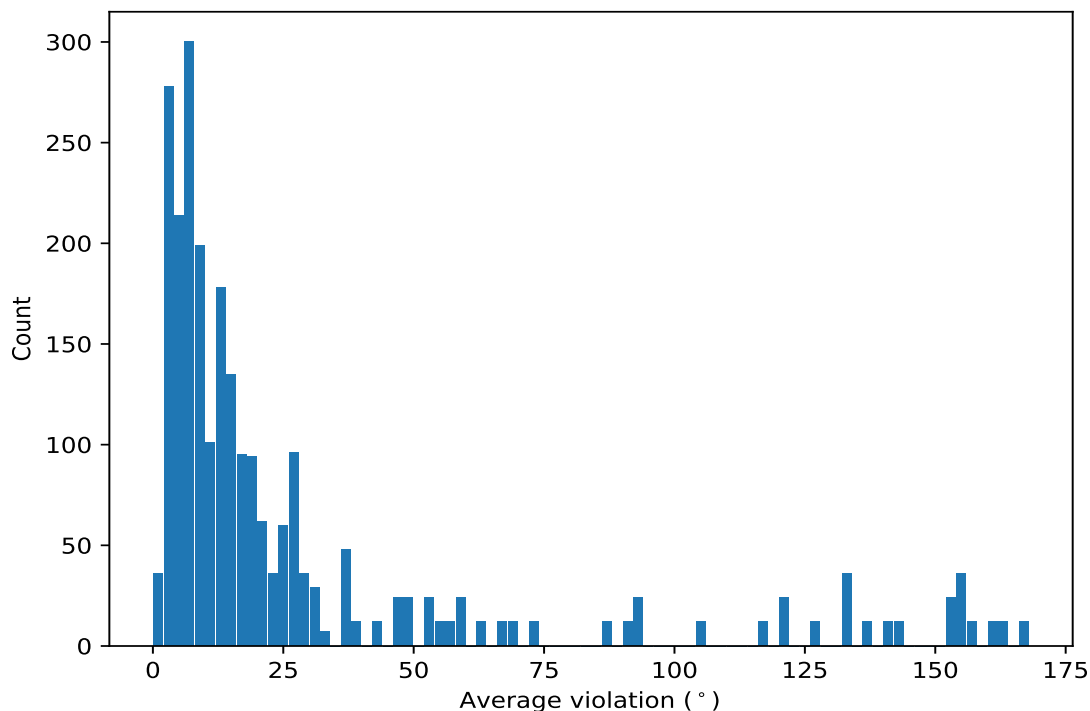
9.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



9.4 Most violated dihedral-angle restraints in the ensemble [i](#)

9.4.1 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



9.4.2 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.

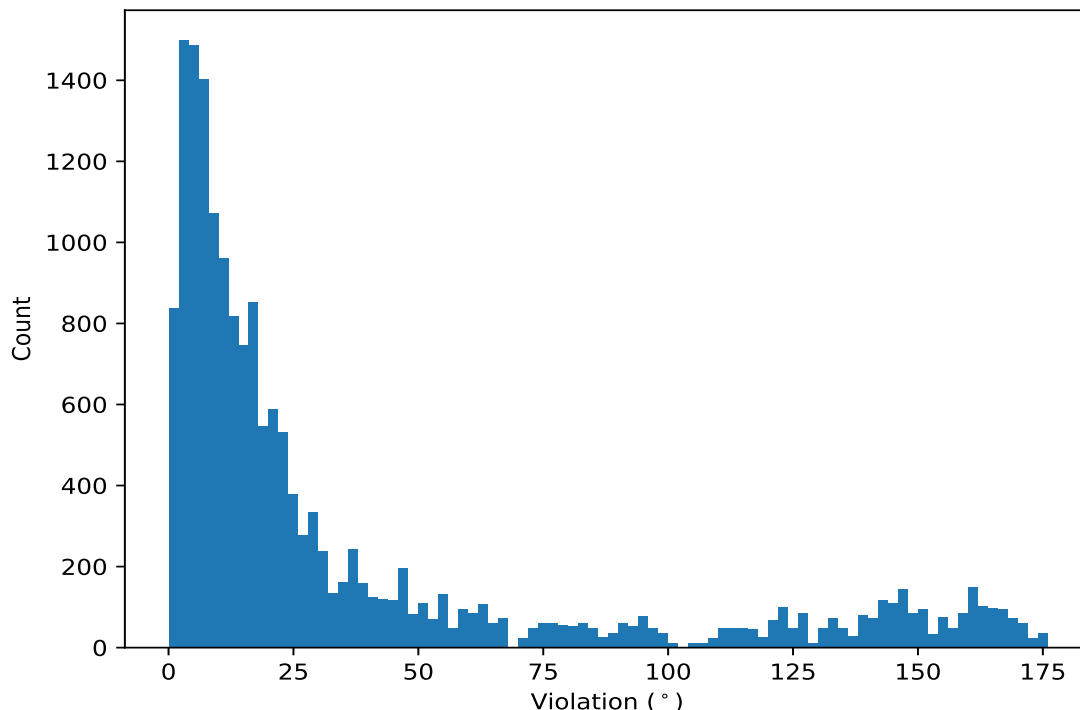
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,2548)	1:L:151:VAL:C	1:L:152:ASN:N	1:L:152:ASN:CA	1:L:152:ASN:C	10	166.82	9.33	171.45
(1,2549)	1:E:151:VAL:C	1:E:152:ASN:N	1:E:152:ASN:CA	1:E:152:ASN:C	10	166.82	9.33	171.45
(1,2550)	1:J:151:VAL:C	1:J:152:ASN:N	1:J:152:ASN:CA	1:J:152:ASN:C	10	166.82	9.35	171.45
(1,2551)	1:H:151:VAL:C	1:H:152:ASN:N	1:H:152:ASN:CA	1:H:152:ASN:C	10	166.82	9.35	171.45
(1,2545)	1:D:151:VAL:C	1:D:152:ASN:N	1:D:152:ASN:CA	1:D:152:ASN:C	10	166.81	9.34	171.45
(1,2546)	1:A:151:VAL:C	1:A:152:ASN:N	1:A:152:ASN:CA	1:A:152:ASN:C	10	166.81	9.36	171.5
(1,2547)	1:K:151:VAL:C	1:K:152:ASN:N	1:K:152:ASN:CA	1:K:152:ASN:C	10	166.81	9.37	171.45
(1,2552)	1:F:151:VAL:C	1:F:152:ASN:N	1:F:152:ASN:CA	1:F:152:ASN:C	10	166.81	9.35	171.45
(1,2553)	1:G:151:VAL:C	1:G:152:ASN:N	1:G:152:ASN:CA	1:G:152:ASN:C	10	166.8	9.36	171.45
(1,2555)	1:B:151:VAL:C	1:B:152:ASN:N	1:B:152:ASN:CA	1:B:152:ASN:C	10	166.8	9.34	171.4

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

9.5 All violated dihedral-angle restraints [i](#)

9.5.1 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.



9.5.2 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 (°)
(1,2555)	1:B:151:VAL:C	1:B:152:ASN:N	1:B:152:ASN:CA	1:B:152:ASN:C	5	174.9
(1,2553)	1:G:151:VAL:C	1:G:152:ASN:N	1:G:152:ASN:CA	1:G:152:ASN:C	5	174.9
(1,2551)	1:H:151:VAL:C	1:H:152:ASN:N	1:H:152:ASN:CA	1:H:152:ASN:C	5	174.9
(1,2550)	1:J:151:VAL:C	1:J:152:ASN:N	1:J:152:ASN:CA	1:J:152:ASN:C	5	174.9
(1,2549)	1:E:151:VAL:C	1:E:152:ASN:N	1:E:152:ASN:CA	1:E:152:ASN:C	5	174.9
(1,2547)	1:K:151:VAL:C	1:K:152:ASN:N	1:K:152:ASN:CA	1:K:152:ASN:C	9	174.9
(1,2545)	1:D:151:VAL:C	1:D:152:ASN:N	1:D:152:ASN:CA	1:D:152:ASN:C	5	174.9
(1,2556)	1:I:151:VAL:C	1:I:152:ASN:N	1:I:152:ASN:CA	1:I:152:ASN:C	5	174.8
(1,2556)	1:I:151:VAL:C	1:I:152:ASN:N	1:I:152:ASN:CA	1:I:152:ASN:C	9	174.8
(1,2555)	1:B:151:VAL:C	1:B:152:ASN:N	1:B:152:ASN:CA	1:B:152:ASN:C	9	174.8