



wwPDB NMR Structure Validation Summary Report ⓘ

Jun 6, 2023 – 05:00 pm BST

PDB ID : 6YJ0
BMRB ID : 50015
Title : Solution NMR structure of titin N2A region Ig domain I83
Authors : Pfuhl, M.; Gage, M.
Deposited on : 2020-04-02

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 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

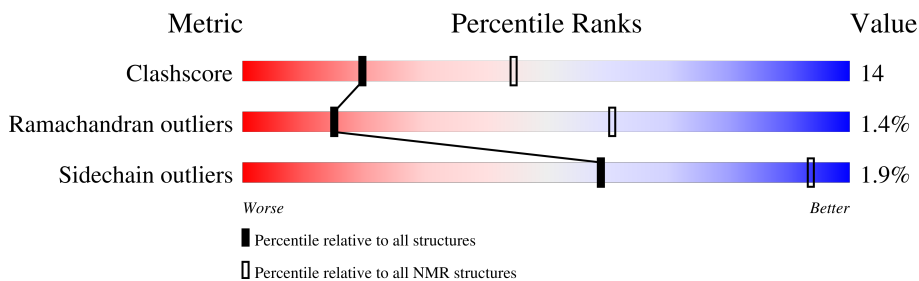
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 92%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	105	

2 Ensemble composition and analysis i

This entry contains 40 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:11-A:83, A:91-A:100 (83)	0.14	14

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 7 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 11, 14, 18, 20, 21, 22, 23, 25, 29, 30, 32, 35, 36, 37, 39
2	3, 8, 10, 12, 13, 16, 19, 26, 33, 40
3	27, 31, 38
4	2, 24
5	5, 17
6	4, 9
7	6, 7
Single-model clusters	15; 28; 34

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1632 atoms, of which 795 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Titin.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	105	1632	520	795	145	168	4	0

There are 14 discrepancies between the modelled and reference sequences:

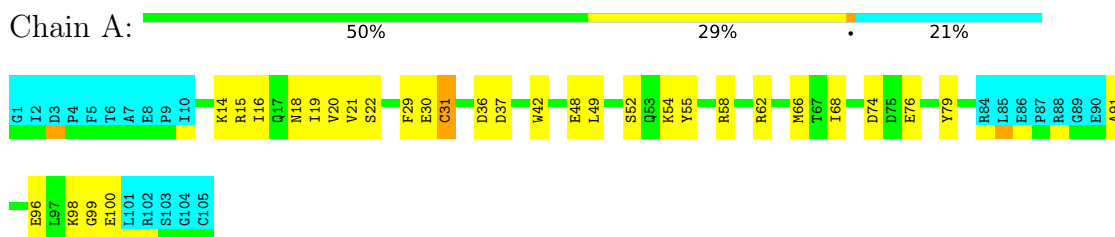
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A2ASS6
A	2	ILE	-	expression tag	UNP A2ASS6
A	3	ASP	-	expression tag	UNP A2ASS6
A	4	PRO	-	expression tag	UNP A2ASS6
A	5	PHE	-	expression tag	UNP A2ASS6
A	6	THR	-	expression tag	UNP A2ASS6
A	98	LYS	-	expression tag	UNP A2ASS6
A	99	GLY	-	expression tag	UNP A2ASS6
A	100	GLU	-	expression tag	UNP A2ASS6
A	101	LEU	-	expression tag	UNP A2ASS6
A	102	ARG	-	expression tag	UNP A2ASS6
A	103	SER	-	expression tag	UNP A2ASS6
A	104	GLY	-	expression tag	UNP A2ASS6
A	105	CYS	-	expression tag	UNP A2ASS6

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.

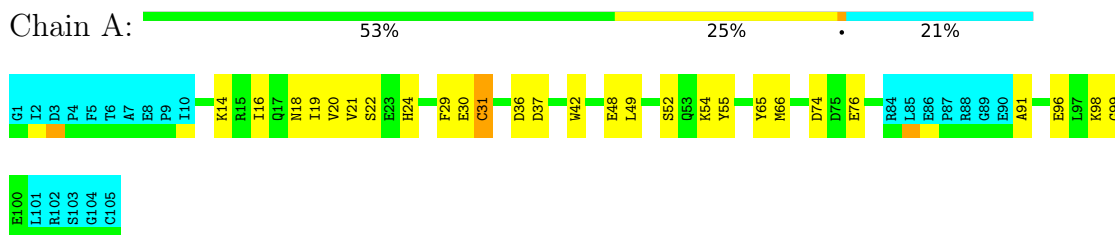
- Molecule 1: Titin



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

The representative model is number 14. Colouring as in section 4.1 above.

- Molecule 1: Titin



5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 40 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
ARIA	structure calculation	2.3.2
X-PLOR NIH	structure calculation	2.35

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	1270
Number of shifts mapped to atoms	1270
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.73±0.01	0±0/683 (0.0± 0.0%)	0.88±0.01	0±0/927 (0.0± 0.0%)
All	All	0.73	0/27320 (0.0%)	0.88	1/37080 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.8±1.9
All	All	0	71

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	65	TYR	CB-CG-CD2	-5.28	117.83	121.00	14	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	58	ARG	Sidechain	19
1	A	62	ARG	Sidechain	18
1	A	15	ARG	Sidechain	17
1	A	92	ARG	Sidechain	17

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	668	627	627	18±2
All	All	26720	25080	25080	722

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 14.

5 of 75 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:TRP:CG	1:A:66:MET:SD	0.64	2.90	31	24
1:A:24:HIS:CE1	1:A:25:GLN:HE21	0.63	2.12	3	1
1:A:48:GLU:H	1:A:48:GLU:CD	0.62	1.97	1	40
1:A:39:ILE:HD12	1:A:39:ILE:N	0.61	2.10	11	4
1:A:43:TYR:CE1	1:A:82:ILE:HD12	0.60	2.31	26	12

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	83/105 (79%)	77±1 (92±1%)	5±1 (6±1%)	1±0 (1±0%)	15	61
All	All	3320/4200 (79%)	3061 (92%)	212 (6%)	47 (1%)	15	61

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	16	ILE	40
1	A	15	ARG	5
1	A	25	GLN	2

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	74/92 (80%)	73±1 (98±1%)	1±1 (2±1%)	59	93
All	All	2960/3680 (80%)	2905 (98%)	55 (2%)	59	93

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	31	CYS	40
1	A	72	THR	10
1	A	48	GLU	5

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

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 92% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_output*

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	1270
Number of shifts mapped to atoms	1270
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](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	103	0.13 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	97	-0.12 ± 0.25	None needed (< 0.5 ppm)
$^{13}\text{C}'$	96	0.04 ± 0.11	None needed (< 0.5 ppm)
^{15}N	97	0.11 ± 0.20	None needed (< 0.5 ppm)

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 92%, i.e. 1018 atoms were assigned a chemical shift out of a possible 1109. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	407/415 (98%)	167/168 (99%)	160/166 (96%)	80/81 (99%)
Sidechain	525/585 (90%)	354/376 (94%)	164/185 (89%)	7/24 (29%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	86/109 (79%)	45/54 (83%)	40/51 (78%)	1/4 (25%)
Overall	1018/1109 (92%)	566/598 (95%)	364/402 (91%)	88/109 (81%)

7.1.4 Statistically unusual chemical shifts [i](#)

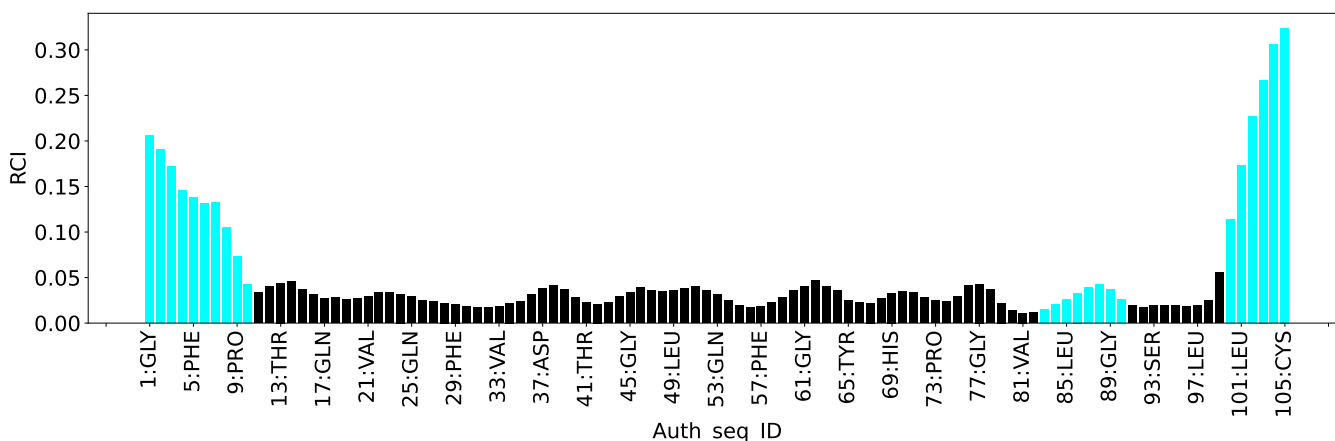
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	66	MET	HB3	-0.28	0.33 – 3.66	-6.8

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	6441
Intra-residue ($ i-j =0$)	3178
Sequential ($ i-j =1$)	1234
Medium range ($ i-j >1$ and $ i-j <5$)	314
Long range ($ i-j \geq 5$)	1715
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	189
Number of unmapped restraints	0
Number of restraints per residue	63.1
Number of long range restraints per residue ¹	16.3

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

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	408.0	0.2
0.2-0.5 (Medium)	164.3	0.5
>0.5 (Large)	7.2	3.29

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)	22.8	6.1
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis [\(i\)](#)

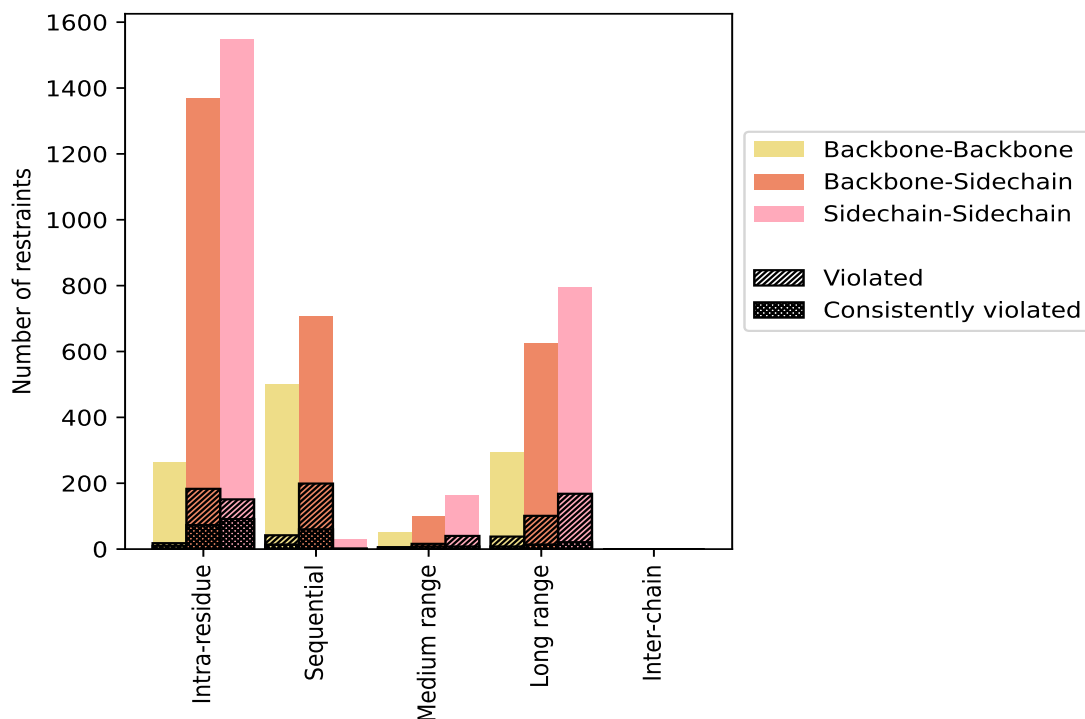
9.1 Summary of distance violations [\(i\)](#)

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	3178	49.3	352	11.1	5.5	174	5.5	2.7
Backbone-Backbone	262	4.1	18	6.9	0.3	10	3.8	0.2
Backbone-Sidechain	1368	21.2	183	13.4	2.8	73	5.3	1.1
Sidechain-Sidechain	1548	24.0	151	9.8	2.3	91	5.9	1.4
Sequential ($i-j =1$)	1234	19.2	243	19.7	3.8	74	6.0	1.1
Backbone-Backbone	499	7.7	42	8.4	0.7	14	2.8	0.2
Backbone-Sidechain	707	11.0	199	28.1	3.1	60	8.5	0.9
Sidechain-Sidechain	28	0.4	2	7.1	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	314	4.9	62	19.7	1.0	17	5.4	0.3
Backbone-Backbone	50	0.8	6	12.0	0.1	1	2.0	0.0
Backbone-Sidechain	100	1.6	16	16.0	0.2	8	8.0	0.1
Sidechain-Sidechain	164	2.5	40	24.4	0.6	8	4.9	0.1
Long range ($i-j \geq 5$)	1715	26.6	307	17.9	4.8	43	2.5	0.7
Backbone-Backbone	295	4.6	38	12.9	0.6	8	2.7	0.1
Backbone-Sidechain	626	9.7	101	16.1	1.6	14	2.2	0.2
Sidechain-Sidechain	794	12.3	168	21.2	2.6	21	2.6	0.3
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	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	6441	100.0	964	15.0	15.0	308	4.8	4.8
Backbone-Backbone	1106	17.2	104	9.4	1.6	33	3.0	0.5
Backbone-Sidechain	2801	43.5	499	17.8	7.7	155	5.5	2.4
Sidechain-Sidechain	2534	39.3	361	14.2	5.6	120	4.7	1.9

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	235	159	36	155	0	585	0.21	3.23	0.23	0.17
2	241	152	35	138	0	566	0.21	3.2	0.25	0.17
3	227	156	35	160	0	578	0.2	3.27	0.2	0.17
4	243	158	38	149	0	588	0.2	3.22	0.23	0.17
5	243	156	36	156	0	591	0.21	3.23	0.23	0.18
6	249	154	33	146	0	582	0.21	3.24	0.23	0.17
7	247	147	39	142	0	575	0.2	3.24	0.23	0.17
8	243	164	38	148	0	593	0.21	3.22	0.22	0.18
9	235	146	35	150	0	566	0.21	3.26	0.25	0.17
10	243	152	37	152	0	584	0.21	3.24	0.23	0.17
11	237	159	39	158	0	593	0.21	3.26	0.23	0.18

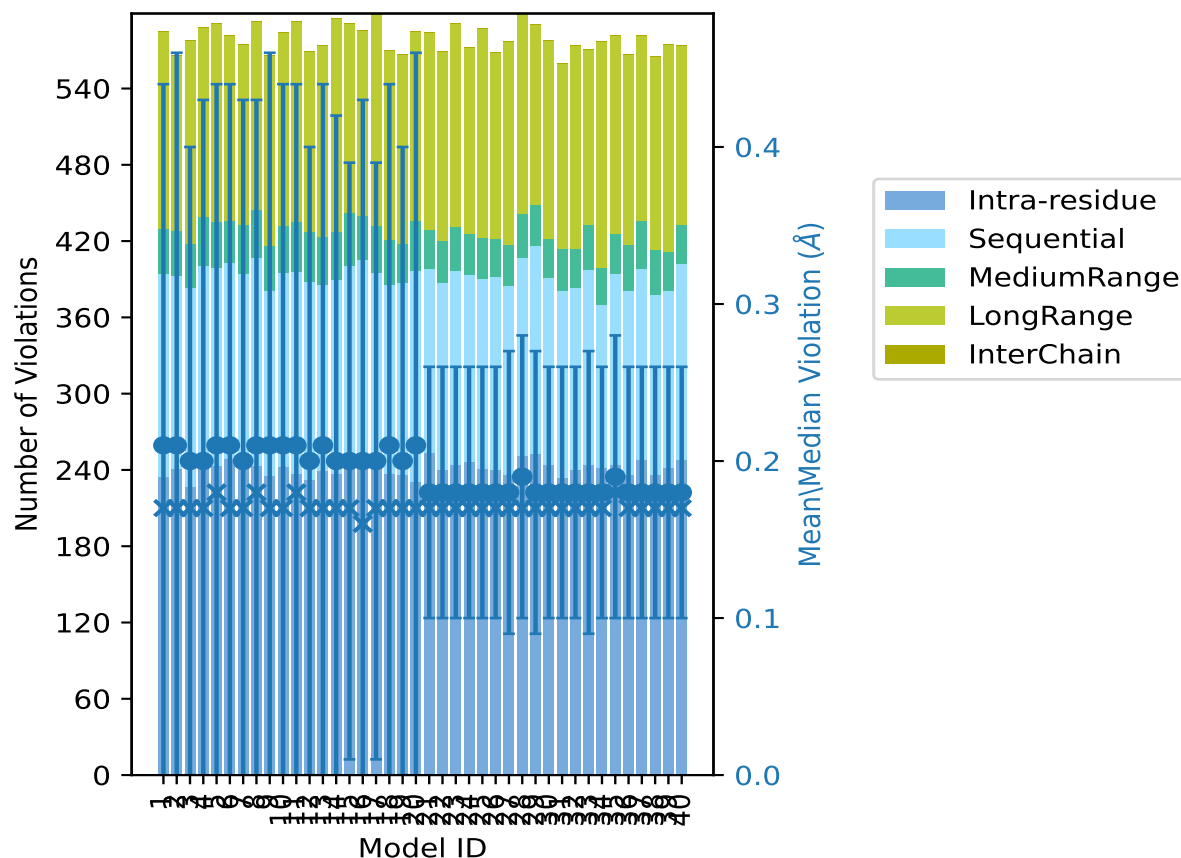
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
12	232	156	39	142	0	569	0.2	3.26	0.2	0.17
13	239	147	37	151	0	574	0.21	3.26	0.23	0.17
14	237	153	37	168	0	595	0.2	3.24	0.22	0.17
15	249	152	41	149	0	591	0.2	3.24	0.19	0.17
16	241	164	35	146	0	586	0.2	3.29	0.23	0.16
17	242	153	37	166	0	598	0.2	3.24	0.19	0.17
18	237	149	35	149	0	570	0.21	3.27	0.23	0.17
19	236	151	31	149	0	567	0.2	3.27	0.2	0.17
20	231	166	39	149	0	585	0.21	3.23	0.25	0.17
21	254	144	31	155	0	584	0.18	1.46	0.08	0.17
22	240	147	33	149	0	569	0.18	1.53	0.08	0.17
23	244	153	34	160	0	591	0.18	1.56	0.08	0.17
24	246	147	33	146	0	572	0.18	1.46	0.08	0.17
25	241	149	33	164	0	587	0.18	1.49	0.08	0.17
26	240	152	30	146	0	568	0.18	1.53	0.08	0.17
27	236	149	32	160	0	577	0.18	1.51	0.09	0.17
28	251	156	34	158	0	599	0.19	1.52	0.09	0.17
29	253	163	33	141	0	590	0.18	1.61	0.09	0.17
30	244	147	31	156	0	578	0.18	1.5	0.08	0.17
31	234	147	33	146	0	560	0.18	1.53	0.08	0.17
32	240	143	31	160	0	574	0.18	1.47	0.08	0.17
33	244	153	36	138	0	571	0.18	1.57	0.09	0.17
34	242	128	29	178	0	577	0.18	1.49	0.08	0.17
35	244	150	32	156	0	582	0.19	1.54	0.09	0.18
36	236	145	36	150	0	567	0.18	1.53	0.08	0.17
37	248	150	38	146	0	582	0.18	1.55	0.08	0.17
38	236	142	35	152	0	565	0.18	1.48	0.08	0.17
39	242	139	31	163	0	575	0.18	1.49	0.08	0.17
40	248	154	31	141	0	574	0.18	1.51	0.08	0.17

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,
⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 5477(IR:2826, SQ:991, MR:252, LR:1408, 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	%
26	25	0	34	0	85	1	2.5
18	8	4	14	0	44	2	5.0
10	6	2	12	0	30	3	7.5
4	8	3	16	0	31	4	10.0
8	10	2	16	0	36	5	12.5
11	6	4	3	0	24	6	15.0

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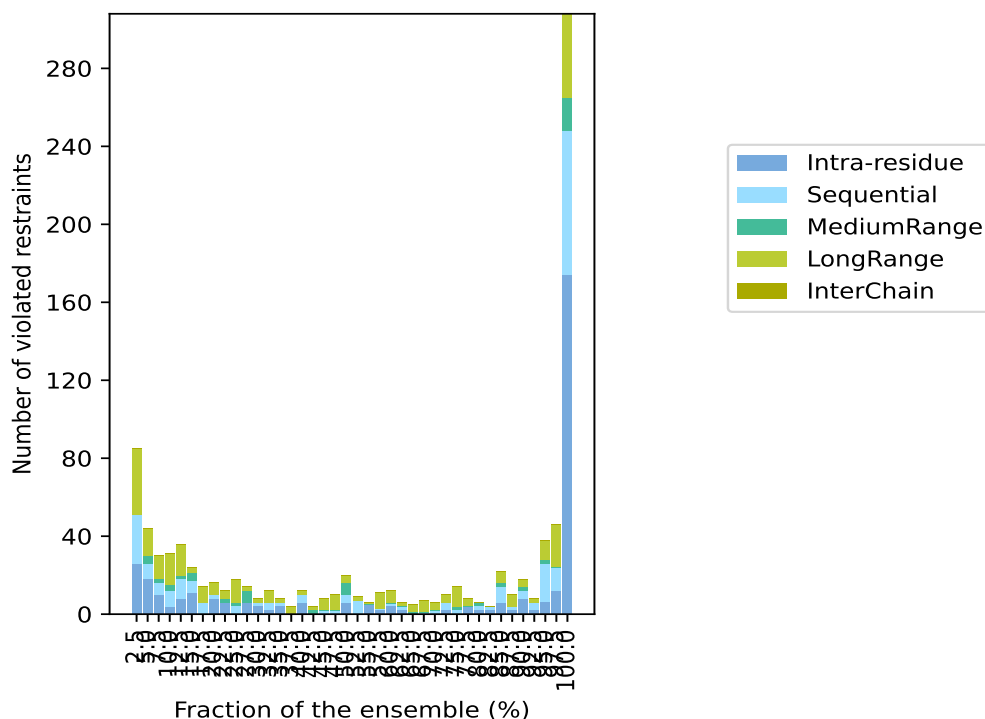
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	6	0	8	0	14	7	17.5
8	2	0	6	0	16	8	20.0
6	0	2	4	0	12	9	22.5
0	4	2	12	0	18	10	25.0
6	0	6	2	0	14	11	27.5
4	2	0	2	0	8	12	30.0
2	4	0	6	0	12	13	32.5
4	2	0	2	0	8	14	35.0
0	0	0	4	0	4	15	37.5
6	4	0	2	0	12	16	40.0
0	0	2	2	0	4	17	42.5
0	2	0	6	0	8	18	45.0
0	2	0	8	0	10	19	47.5
6	4	6	4	0	20	20	50.0
0	7	0	2	0	9	21	52.5
5	0	0	1	0	6	22	55.0
2	1	0	8	0	11	23	57.5
4	1	1	6	0	12	24	60.0
2	2	0	2	0	6	25	62.5
0	0	1	4	0	5	26	65.0
0	1	0	6	0	7	27	67.5
0	2	0	4	0	6	28	70.0
2	4	0	4	0	10	29	72.5
0	2	2	10	0	14	30	75.0
4	0	0	4	0	8	31	77.5
2	2	2	0	0	6	32	80.0
2	2	0	0	0	4	33	82.5
6	8	2	6	0	22	34	85.0
2	2	0	6	0	10	35	87.5
8	4	2	4	0	18	36	90.0
2	4	0	2	0	8	37	92.5
6	20	2	10	0	38	38	95.0
12	12	0	22	0	46	39	97.5
174	74	17	43	0	308	40	100.0

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

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

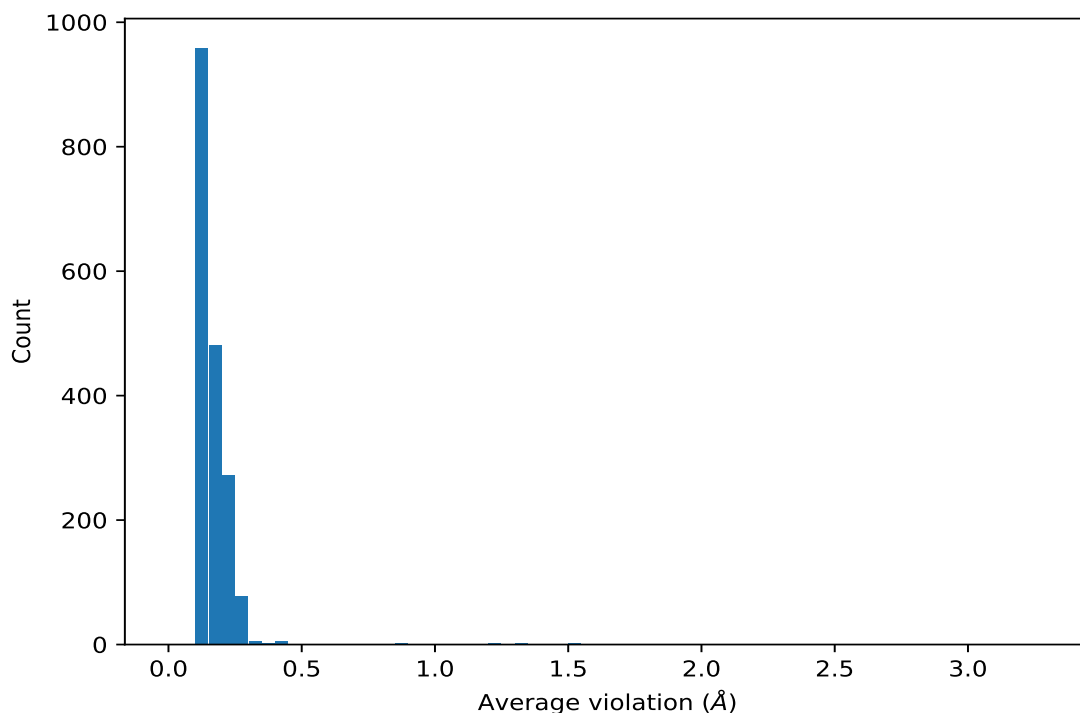
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,1673)	1:A:85:LEU:HD21	1:A:88:ARG:HG3	40	1.52	0.03	1.52
(3,1673)	1:A:85:LEU:HD22	1:A:88:ARG:HG3	40	1.52	0.03	1.52
(3,1673)	1:A:85:LEU:HD23	1:A:88:ARG:HG3	40	1.52	0.03	1.52
(3,2069)	1:A:85:LEU:HD11	1:A:88:ARG:HG3	40	0.87	0.1	0.88
(3,2069)	1:A:85:LEU:HD12	1:A:88:ARG:HG3	40	0.87	0.1	0.88
(3,2069)	1:A:85:LEU:HD13	1:A:88:ARG:HG3	40	0.87	0.1	0.88
(3,37)	1:A:88:ARG:H	1:A:88:ARG:HG2	40	0.51	0.04	0.52
(3,1353)	1:A:16:ILE:HD11	1:A:17:GLN:H	40	0.41	0.02	0.41
(3,1353)	1:A:16:ILE:HD12	1:A:17:GLN:H	40	0.41	0.02	0.41
(3,1353)	1:A:16:ILE:HD13	1:A:17:GLN:H	40	0.41	0.02	0.41
(3,563)	1:A:47:THR:H	1:A:45:GLY:HA2	40	0.39	0.05	0.39
(3,2649)	1:A:9:PRO:HB3	1:A:9:PRO:HD3	40	0.39	0.06	0.4
(1,1669)	1:A:85:LEU:HD21	1:A:88:ARG:HG3	40	0.32	0.03	0.32
(1,1669)	1:A:85:LEU:HD22	1:A:88:ARG:HG3	40	0.32	0.03	0.32
(1,1669)	1:A:85:LEU:HD23	1:A:88:ARG:HG3	40	0.32	0.03	0.32
(1,123)	1:A:55:TYR:H	1:A:54:LYS:H	40	0.3	0.02	0.3

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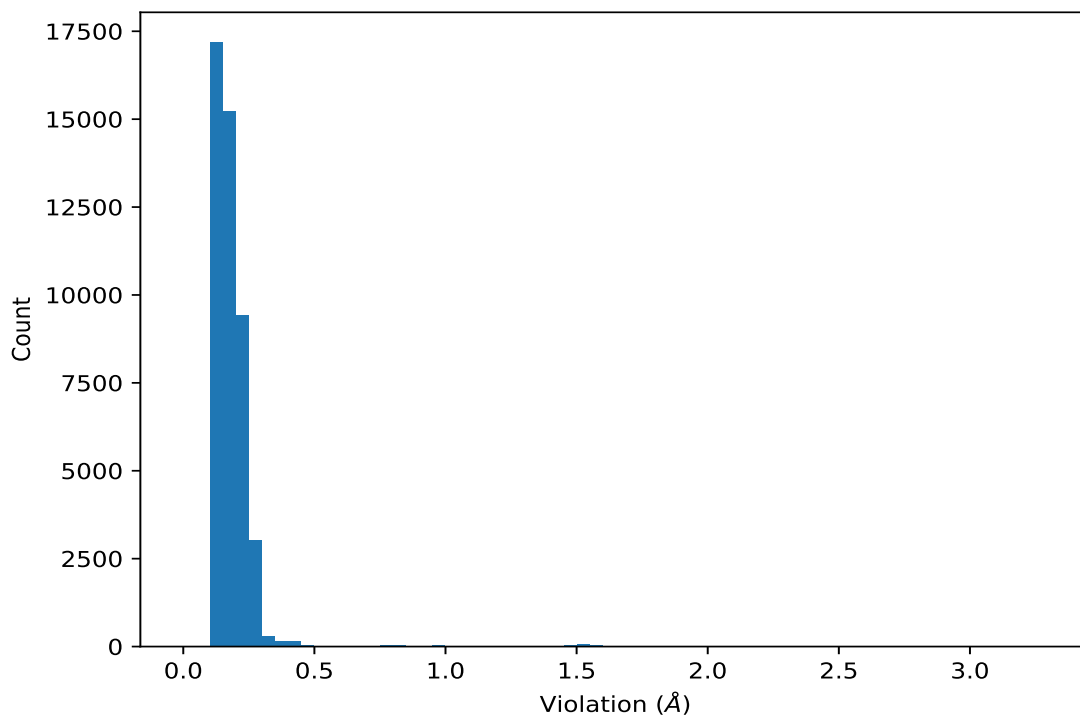
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,125)	1:A:55:TYR:H	1:A:54:LYS:H	40	0.3	0.02	0.3
(3,2485)	1:A:9:PRO:HD3	1:A:9:PRO:HB3	40	0.29	0.06	0.31

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,34)	1:A:88:ARG:H	1:A:86:GLU:HA	16	3.29
(3,34)	1:A:88:ARG:H	1:A:86:GLU:HA	3	3.27
(3,34)	1:A:88:ARG:H	1:A:86:GLU:HA	18	3.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,34)	1:A:88:ARG:H	1:A:86:GLU:HA	19	3.27
(3,34)	1:A:88:ARG:H	1:A:86:GLU:HA	9	3.26
(3,34)	1:A:88:ARG:H	1:A:86:GLU:HA	11	3.26
(3,34)	1:A:88:ARG:H	1:A:86:GLU:HA	12	3.26
(3,34)	1:A:88:ARG:H	1:A:86:GLU:HA	13	3.26
(3,34)	1:A:88:ARG:H	1:A:86:GLU:HA	6	3.24
(3,34)	1:A:88:ARG:H	1:A:86:GLU:HA	7	3.24

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

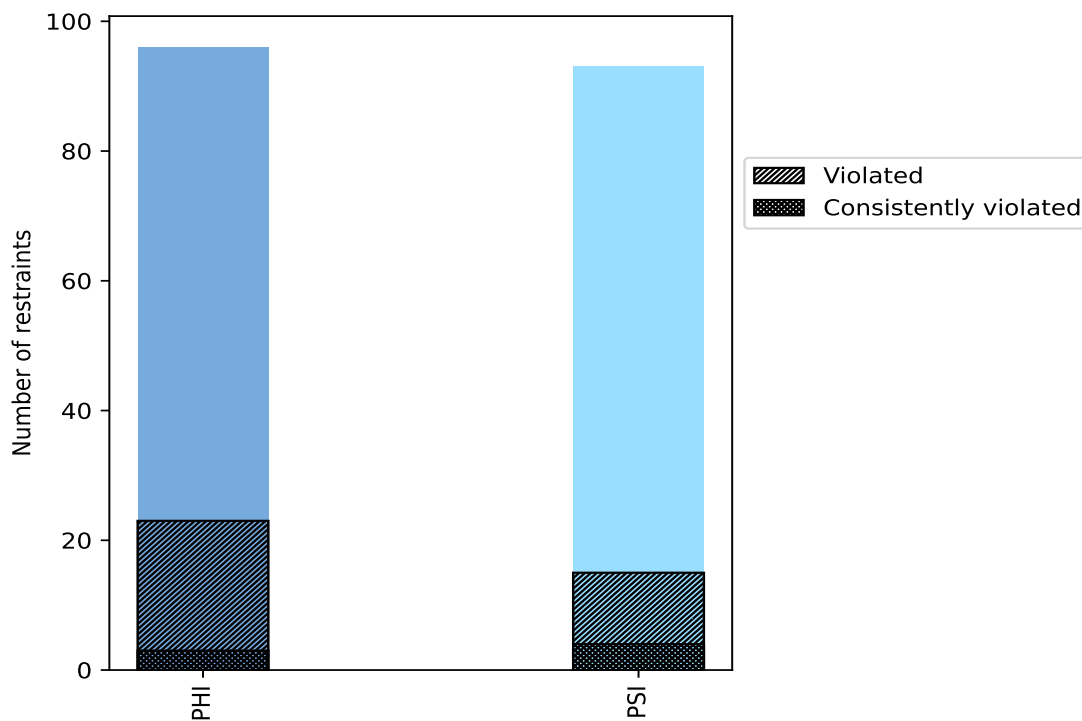
10.1 Summary of dihedral-angle violations [i](#)

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	96	50.8	23	24.0	12.2	3	3.1	1.6
PSI	93	49.2	15	16.1	7.9	4	4.3	2.1
Total	189	100.0	38	20.1	20.1	7	3.7	3.7

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

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



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

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

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

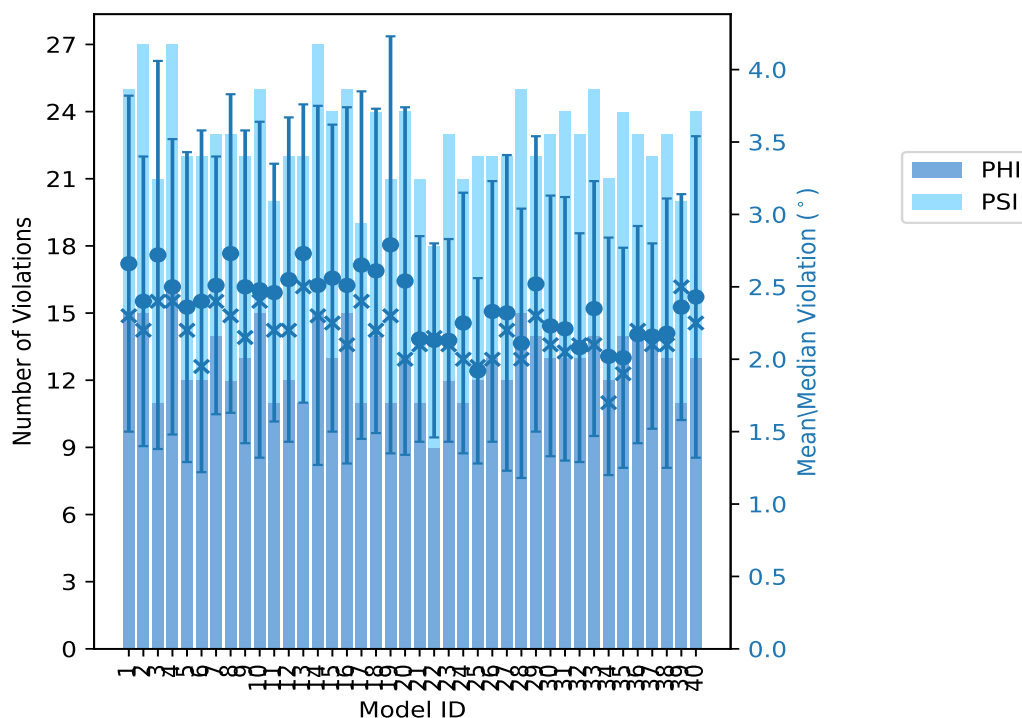
Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	15	10	25	2.66	4.9	1.16	2.3
2	15	12	27	2.4	4.8	1.0	2.2
3	11	10	21	2.72	6.1	1.34	2.4
4	16	11	27	2.5	4.9	1.02	2.4
5	12	10	22	2.36	5.0	1.07	2.2
6	12	10	22	2.4	5.3	1.18	1.95
7	14	9	23	2.51	4.9	0.89	2.4
8	12	11	23	2.73	5.3	1.1	2.3
9	13	9	22	2.5	4.8	1.08	2.15
10	15	10	25	2.48	4.9	1.16	2.4
11	11	9	20	2.46	4.4	0.89	2.2
12	12	10	22	2.55	5.0	1.12	2.2
13	11	11	22	2.73	4.9	1.03	2.5
14	15	12	27	2.51	6.1	1.24	2.3
15	13	11	24	2.56	5.0	1.06	2.25
16	15	10	25	2.51	6.0	1.23	2.1
17	11	8	19	2.65	5.9	1.2	2.4
18	14	10	24	2.61	5.4	1.12	2.2
19	11	10	21	2.79	6.0	1.44	2.3
20	13	11	24	2.54	5.1	1.2	2.0
21	11	10	21	2.14	3.8	0.71	2.1
22	9	9	18	2.13	3.5	0.67	2.15
23	12	11	23	2.13	3.4	0.7	2.1
24	11	10	21	2.25	4.6	0.9	2.0
25	12	10	22	1.92	3.2	0.64	1.95
26	13	9	22	2.33	5.2	0.9	2.0
27	12	10	22	2.32	5.8	1.09	2.2
28	15	10	25	2.11	5.1	0.93	2.0
29	14	8	22	2.52	5.3	1.02	2.3
30	13	10	23	2.23	5.1	0.9	2.1
31	13	11	24	2.21	5.1	0.91	2.05
32	13	10	23	2.08	4.1	0.79	2.1
33	14	11	25	2.35	5.2	0.88	2.1
34	12	9	21	2.02	3.8	0.82	1.7
35	14	10	24	2.01	3.6	0.76	1.9
36	14	9	23	2.17	3.8	0.75	2.2
37	14	8	22	2.16	3.5	0.64	2.1
38	13	10	23	2.18	5.2	0.93	2.1

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Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
39	11	9	20	2.36	3.5	0.78	2.5
40	13	11	24	2.43	5.5	1.11	2.25

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
3	2	5	1	2.5
1	0	1	2	5.0
0	0	0	3	7.5
1	1	2	4	10.0

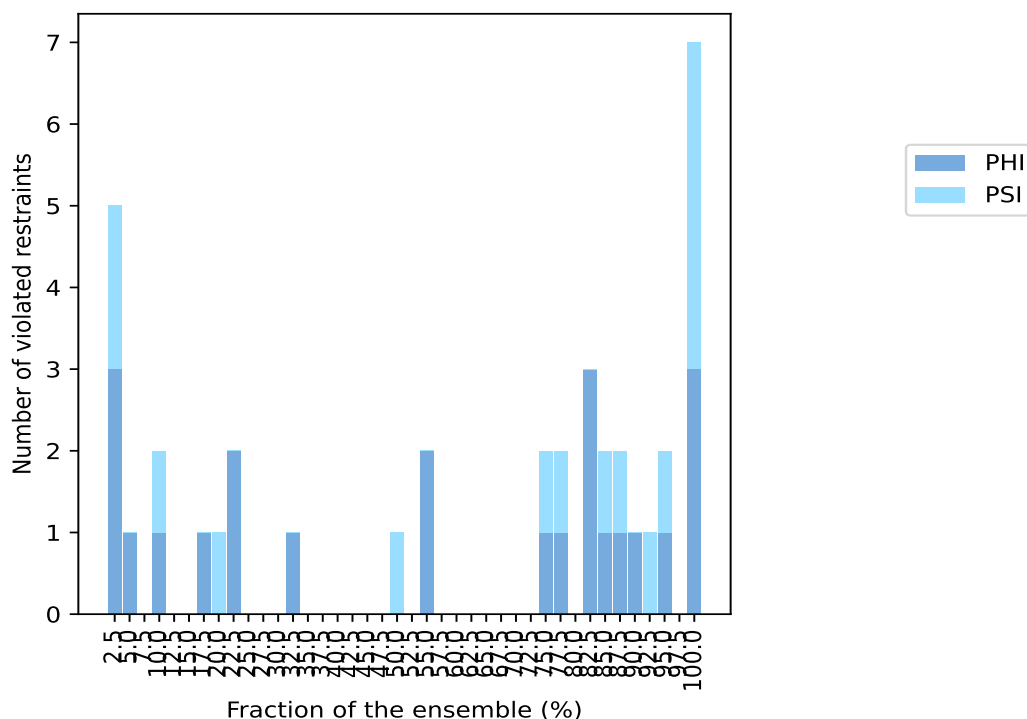
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	5	12.5
0	0	0	6	15.0
1	0	1	7	17.5
0	1	1	8	20.0
2	0	2	9	22.5
0	0	0	10	25.0
0	0	0	11	27.5
0	0	0	12	30.0
1	0	1	13	32.5
0	0	0	14	35.0
0	0	0	15	37.5
0	0	0	16	40.0
0	0	0	17	42.5
0	0	0	18	45.0
0	0	0	19	47.5
0	1	1	20	50.0
0	0	0	21	52.5
2	0	2	22	55.0
0	0	0	23	57.5
0	0	0	24	60.0
0	0	0	25	62.5
0	0	0	26	65.0
0	0	0	27	67.5
0	0	0	28	70.0
0	0	0	29	72.5
1	1	2	30	75.0
1	1	2	31	77.5
0	0	0	32	80.0
3	0	3	33	82.5
1	1	2	34	85.0
1	1	2	35	87.5
1	0	1	36	90.0
0	1	1	37	92.5
1	1	2	38	95.0
0	0	0	39	97.5
3	4	7	40	100.0

¹ Number of models with violations

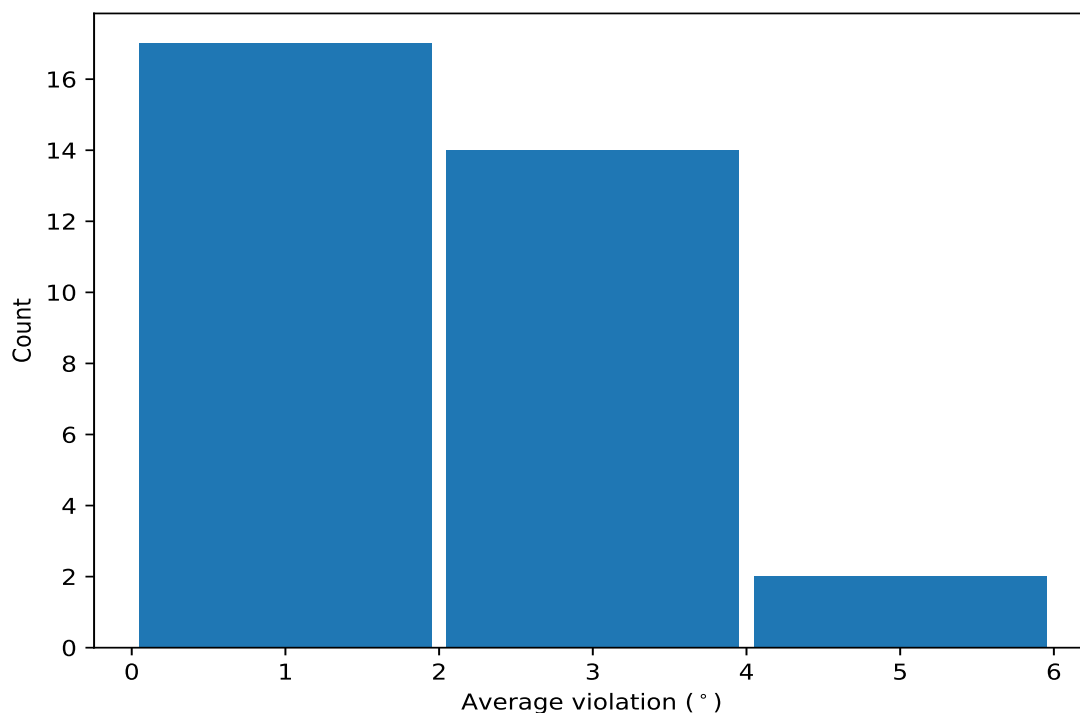
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

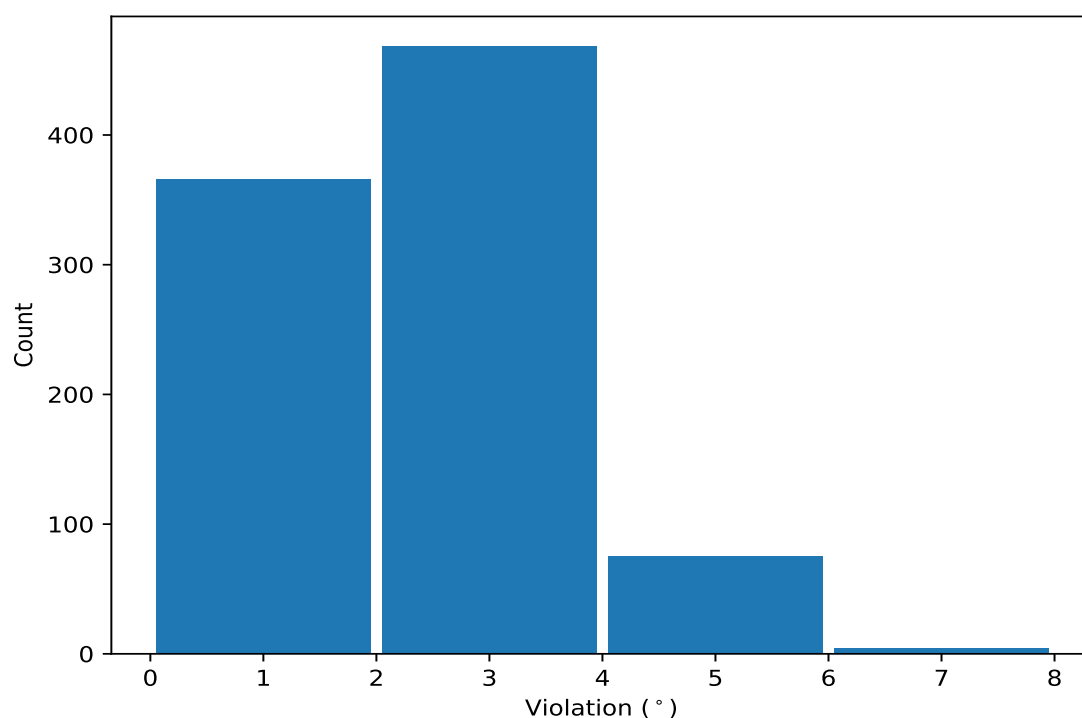
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,20)	1:A:15:ARG:N	1:A:15:ARG:CA	1:A:15:ARG:C	1:A:16:ILE:N	40	3.48	0.39	3.5
(1,63)	1:A:37:ASP:C	1:A:38:ALA:N	1:A:38:ALA:CA	1:A:38:ALA:C	40	3.22	0.57	3.2
(1,58)	1:A:35:PHE:N	1:A:35:PHE:CA	1:A:35:PHE:C	1:A:36:ASP:N	40	2.64	0.67	2.6
(1,71)	1:A:41:THR:C	1:A:42:TRP:N	1:A:42:TRP:CA	1:A:42:TRP:C	40	2.57	0.42	2.5
(1,18)	1:A:14:LYS:N	1:A:14:LYS:CA	1:A:14:LYS:C	1:A:15:ARG:N	40	2.35	0.26	2.4
(1,22)	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	1:A:17:GLN:N	40	2.17	0.28	2.2
(1,21)	1:A:15:ARG:C	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	40	2.17	0.37	2.2
(1,97)	1:A:56:ASN:N	1:A:56:ASN:CA	1:A:56:ASN:C	1:A:57:PHE:N	38	2.35	0.56	2.4
(1,158)	1:A:87:PRO:C	1:A:88:ARG:N	1:A:88:ARG:CA	1:A:88:ARG:C	38	1.7	0.4	1.6
(1,56)	1:A:34:SER:N	1:A:34:SER:CA	1:A:34:SER:C	1:A:35:PHE:N	37	3.25	0.53	3.2

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

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

10.5.1 Histogram : Distribution of violations [i](#)

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



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

The following table provides the list of violations for the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,154)	1:A:85:LEU:C	1:A:86:GLU:N	1:A:86:GLU:CA	1:A:86:GLU:C	14	6.1
(1,153)	1:A:85:LEU:N	1:A:85:LEU:CA	1:A:85:LEU:C	1:A:86:GLU:N	3	6.1
(1,153)	1:A:85:LEU:N	1:A:85:LEU:CA	1:A:85:LEU:C	1:A:86:GLU:N	16	6.0
(1,153)	1:A:85:LEU:N	1:A:85:LEU:CA	1:A:85:LEU:C	1:A:86:GLU:N	19	6.0
(1,154)	1:A:85:LEU:C	1:A:86:GLU:N	1:A:86:GLU:CA	1:A:86:GLU:C	17	5.9
(1,92)	1:A:53:GLN:N	1:A:53:GLN:CA	1:A:53:GLN:C	1:A:54:LYS:N	27	5.8
(1,92)	1:A:53:GLN:N	1:A:53:GLN:CA	1:A:53:GLN:C	1:A:54:LYS:N	3	5.7
(1,92)	1:A:53:GLN:N	1:A:53:GLN:CA	1:A:53:GLN:C	1:A:54:LYS:N	19	5.7
(1,92)	1:A:53:GLN:N	1:A:53:GLN:CA	1:A:53:GLN:C	1:A:54:LYS:N	40	5.5
(1,154)	1:A:85:LEU:C	1:A:86:GLU:N	1:A:86:GLU:CA	1:A:86:GLU:C	18	5.4