



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2LUM / pdb_00002lum
BMRB ID : 18531
Title : Three-State Ensemble obtained from eNOEs of the Third Immunoglobulin Binding Domain of Protein G (GB3)
Authors : Vogeli, B.; Kazemi, S.; Guntert, P.; Riek, R.
Deposited on : 2012-06-18

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

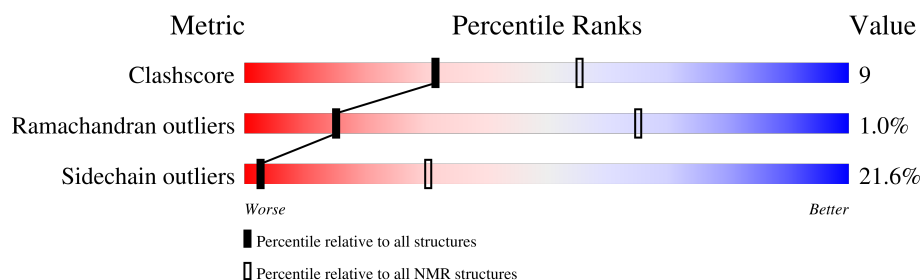
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	56	

2 Ensemble composition and analysis

This entry contains 60 models. Model 25 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:1-A:56 (56)	0.61	25

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters. No single-model clusters were found.

Cluster number	Models
1	21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 34, 35, 36, 37, 38, 39, 40, 49, 53
2	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20
3	33, 41, 42, 43, 44, 45, 46, 47, 48, 50, 51, 52, 54, 55, 56, 57, 58, 59, 60

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 859 atoms, of which 423 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Immunoglobulin G-binding protein G.

Mol	Chain	Residues	Atoms							Trace
1	A	56	Total	C	H	N	O	S		0
			859	274	423	69	92	1		

There are 2 discrepancies between the modelled and reference sequences:

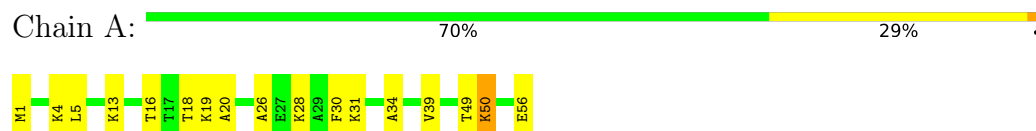
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P19909
A	2	GLN	-	expression tag	UNP P19909

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.

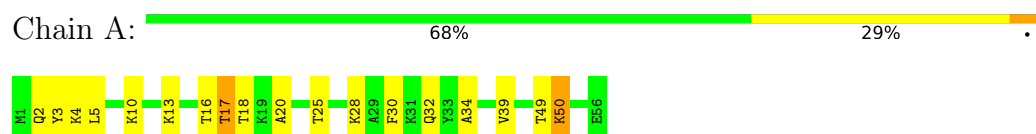
- Molecule 1: Immunoglobulin G-binding protein G



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

The representative model is number 25. Colouring as in section 4.1 above.

- Molecule 1: Immunoglobulin G-binding protein G



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 60 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	refinement	

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	625
Number of shifts mapped to atoms	625
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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	436	423	425	8±3
All	All	26160	25380	25500	451

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 9.

5 of 89 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ALA:HB1	1:A:25:THR:HG23	1.03	1.28	6	12
1:A:20:ALA:HB3	1:A:26:ALA:HB2	0.72	1.60	19	29
1:A:5:LEU:HD22	1:A:30:PHE:CD1	0.69	2.23	28	23
1:A:26:ALA:HB1	1:A:30:PHE:CE2	0.68	2.24	59	4
1:A:49:THR:O	1:A:50:LYS:C	0.66	2.38	51	40

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	54/56 (96%)	49±2 (92±4%)	4±2 (8±3%)	1±1 (1±1%)	15	65
All	All	3240/3360 (96%)	2965 (92%)	243 (8%)	32 (1%)	15	65

All 4 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	50	LYS	18
1	A	39	VAL	6
1	A	2	GLN	5
1	A	53	THR	3

6.3.2 Protein sidechains ⓘ

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	46/46 (100%)	36±3 (78±6%)	10±3 (22±6%)	3	30
All	All	2760/2760 (100%)	2165 (78%)	595 (22%)	3	30

5 of 34 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	50	LYS	51
1	A	28	LYS	41
1	A	19	LYS	40
1	A	1	MET	37
1	A	13	LYS	31

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides 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 86% for the well-defined parts and 86% 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	625
Number of shifts mapped to atoms	625
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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
$^{13}\text{C}_\alpha$	56	-0.20 ± 0.28	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	52	0.09 ± 0.25	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	54	-0.20 ± 0.53	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 86%, i.e. 624 atoms were assigned a chemical shift out of a possible 724. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	225/284 (79%)	115/116 (99%)	56/112 (50%)	54/56 (96%)
Sidechain	344/381 (90%)	242/245 (99%)	102/124 (82%)	0/12 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	55/59 (93%)	28/28 (100%)	27/30 (90%)	0/1 (0%)
Overall	624/724 (86%)	385/389 (99%)	185/266 (70%)	54/69 (78%)

7.1.4 Statistically unusual chemical shifts [i](#)

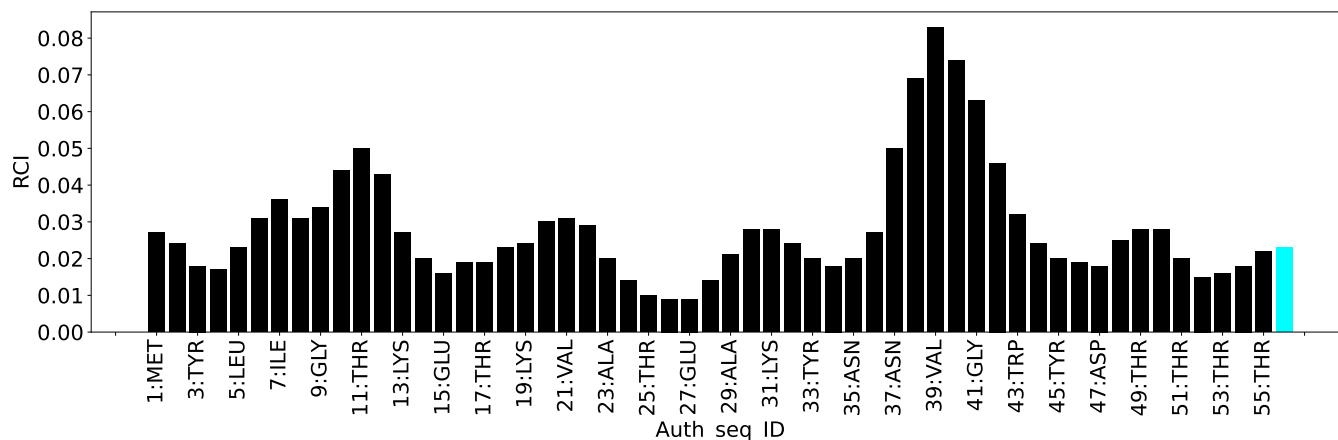
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	5	LEU	HB3	-1.20	-0.26 – 3.31	-7.6
1	A	54	VAL	HB	-0.37	0.43 – 3.54	-7.6

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	5119
Intra-residue ($ i-j =0$)	1593
Sequential ($ i-j =1$)	1441
Medium range ($ i-j >1$ and $ i-j <5$)	723
Long range ($ i-j \geq 5$)	1362
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	59
Number of unmapped restraints	0
Number of restraints per residue	30.8
Number of long range restraints per residue ¹	8.1

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)	76.2	0.2
0.2-0.5 (Medium)	350.9	0.5
>0.5 (Large)	4253.0	9.15

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)	0.6	9.96
10.0-20.0 (Medium)	0.2	15.82
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

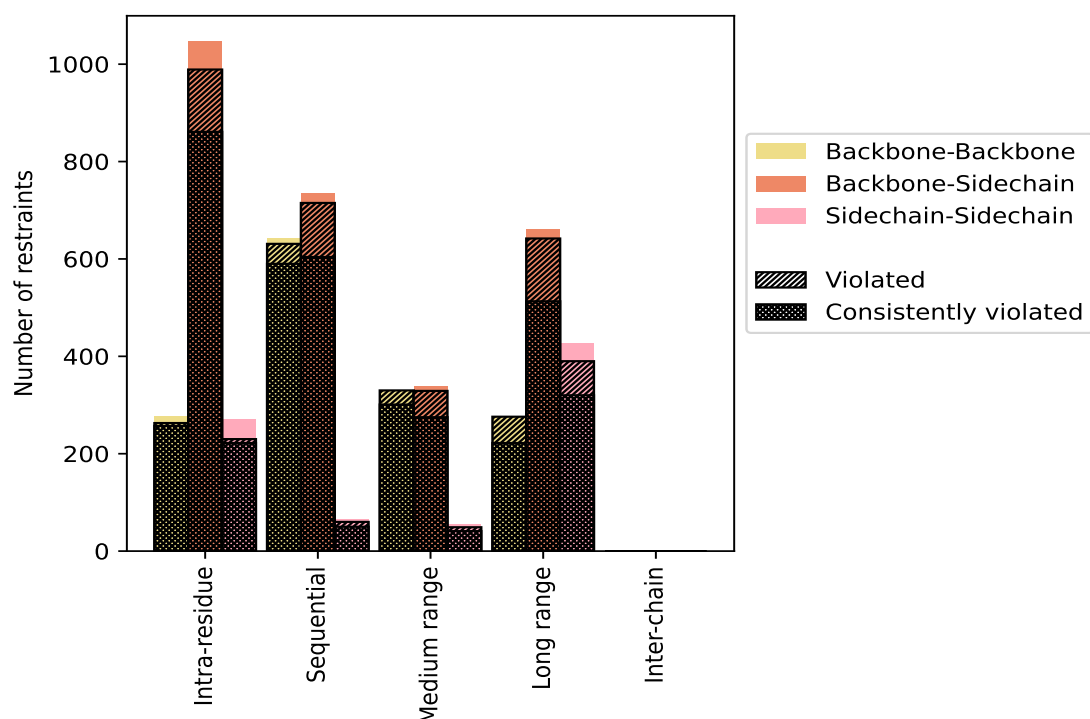
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	1593	31.1	1482	93.0	29.0	1340	84.1	26.2
Backbone-Backbone	276	5.4	263	95.3	5.1	257	93.1	5.0
Backbone-Sidechain	1047	20.5	989	94.5	19.3	861	82.2	16.8
Sidechain-Sidechain	270	5.3	230	85.2	4.5	222	82.2	4.3
Sequential (i-j =1)	1441	28.2	1406	97.6	27.5	1244	86.3	24.3
Backbone-Backbone	642	12.5	631	98.3	12.3	590	91.9	11.5
Backbone-Sidechain	734	14.3	715	97.4	14.0	604	82.3	11.8
Sidechain-Sidechain	65	1.3	60	92.3	1.2	50	76.9	1.0
Medium range (i-j >1 & i-j <5)	723	14.1	708	97.9	13.8	617	85.3	12.1
Backbone-Backbone	330	6.4	330	100.0	6.4	301	91.2	5.9
Backbone-Sidechain	339	6.6	329	97.1	6.4	275	81.1	5.4
Sidechain-Sidechain	54	1.1	49	90.7	1.0	41	75.9	0.8
Long range (i-j ≥5)	1362	26.6	1308	96.0	25.6	1055	77.5	20.6
Backbone-Backbone	276	5.4	276	100.0	5.4	222	80.4	4.3
Backbone-Sidechain	660	12.9	642	97.3	12.5	513	77.7	10.0
Sidechain-Sidechain	426	8.3	390	91.5	7.6	320	75.1	6.3
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	5119	100.0	4904	95.8	95.8	4256	83.1	83.1
Backbone-Backbone	1524	29.8	1500	98.4	29.3	1370	89.9	26.8
Backbone-Sidechain	2780	54.3	2675	96.2	52.3	2253	81.0	44.0
Sidechain-Sidechain	815	15.9	729	89.4	14.2	633	77.7	12.4

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	1428	1350	684	1225	0	4687	2.93	8.42	1.58	2.99
2	1423	1351	678	1228	0	4680	2.93	8.7	1.58	2.97
3	1428	1345	686	1228	0	4687	2.95	8.2	1.59	2.99
4	1423	1345	682	1225	0	4675	2.94	7.43	1.57	2.99
5	1416	1344	686	1213	0	4659	2.98	8.34	1.6	2.99
6	1416	1346	685	1230	0	4677	2.97	8.69	1.61	2.99
7	1424	1347	677	1226	0	4674	2.94	8.88	1.59	2.99
8	1422	1350	681	1223	0	4676	2.91	8.58	1.57	2.99
9	1427	1337	679	1227	0	4670	2.92	8.07	1.57	2.98
10	1423	1336	679	1217	0	4655	2.93	8.09	1.57	2.97

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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1430	1344	684	1224	0	4682	2.96	8.17	1.61	2.99
12	1425	1349	686	1230	0	4690	2.97	8.62	1.61	2.99
13	1424	1341	677	1227	0	4669	2.93	8.94	1.58	2.99
14	1422	1352	679	1234	0	4687	2.95	8.32	1.58	2.99
15	1420	1344	680	1219	0	4663	2.93	7.41	1.57	2.98
16	1433	1347	684	1219	0	4683	2.92	8.02	1.57	2.99
17	1417	1349	685	1230	0	4681	2.95	9.15	1.61	2.98
18	1426	1353	682	1207	0	4668	2.91	7.32	1.56	2.97
19	1423	1345	679	1214	0	4661	2.94	8.94	1.59	2.98
20	1425	1343	683	1244	0	4695	2.97	8.61	1.61	2.99
21	1426	1352	678	1233	0	4689	2.89	7.3	1.55	2.98
22	1433	1355	676	1234	0	4698	2.88	7.35	1.55	2.98
23	1425	1352	669	1227	0	4673	2.91	8.59	1.56	2.99
24	1431	1352	679	1227	0	4689	2.95	8.43	1.61	2.98
25	1433	1351	678	1235	0	4697	2.89	7.75	1.55	2.99
26	1442	1352	680	1226	0	4700	2.88	7.7	1.56	2.98
27	1429	1354	674	1228	0	4685	2.89	7.89	1.56	2.99
28	1433	1355	680	1228	0	4696	2.88	7.76	1.56	2.98
29	1424	1354	678	1224	0	4680	2.93	8.71	1.58	2.98
30	1432	1357	673	1222	0	4684	2.89	7.73	1.56	2.99
31	1433	1352	674	1237	0	4696	2.93	8.38	1.59	2.99
32	1435	1359	675	1228	0	4697	2.89	7.76	1.56	2.99
33	1432	1345	677	1228	0	4682	2.96	8.3	1.59	2.99
34	1431	1347	675	1228	0	4681	2.93	8.4	1.59	2.99
35	1433	1354	680	1233	0	4700	2.96	8.51	1.61	2.99
36	1429	1349	672	1235	0	4685	2.92	7.2	1.56	2.99
37	1426	1350	675	1227	0	4678	2.91	8.6	1.57	2.99
38	1440	1354	676	1232	0	4702	2.9	7.84	1.57	2.99
39	1430	1357	671	1237	0	4695	2.92	7.73	1.58	2.99
40	1432	1360	673	1228	0	4693	2.88	7.63	1.56	2.99
41	1434	1352	678	1219	0	4683	2.96	8.64	1.6	2.99
42	1426	1345	681	1223	0	4675	2.96	7.86	1.59	2.99
43	1429	1355	676	1228	0	4688	2.93	7.91	1.57	2.99
44	1435	1342	676	1235	0	4688	2.94	7.88	1.58	2.99
45	1429	1351	676	1232	0	4688	2.93	7.9	1.58	2.99
46	1430	1346	680	1229	0	4685	2.93	7.89	1.58	2.99
47	1432	1349	679	1240	0	4700	2.95	7.76	1.58	2.99
48	1425	1347	679	1233	0	4684	2.95	7.9	1.58	2.99
49	1435	1345	674	1223	0	4677	2.9	7.78	1.55	2.99
50	1436	1360	681	1245	0	4722	3.03	8.94	1.66	3.01
51	1427	1351	675	1230	0	4683	2.94	7.9	1.57	2.99

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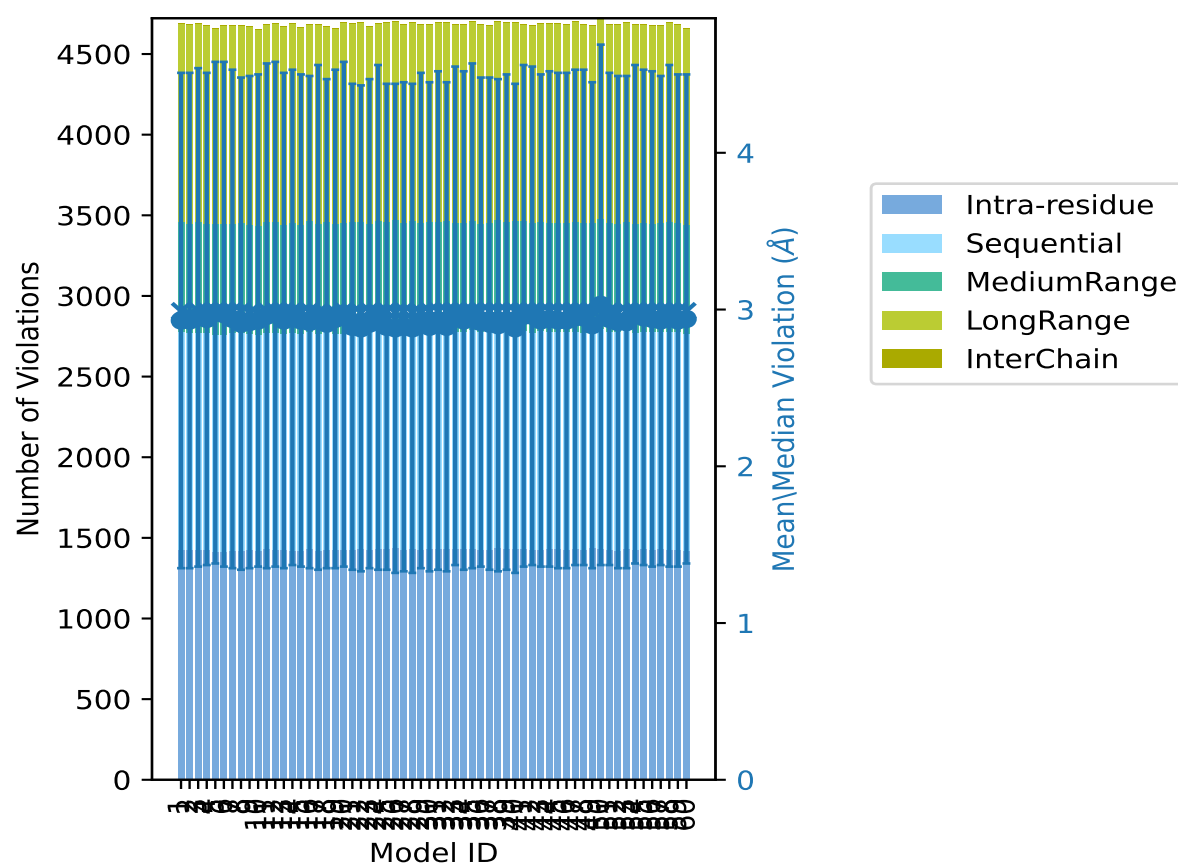
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
52	1424	1353	674	1230	0	4681	2.92	7.81	1.57	2.98
53	1432	1353	675	1233	0	4693	2.92	7.76	1.57	2.99
54	1427	1342	680	1232	0	4681	2.97	7.91	1.59	2.99
55	1432	1347	674	1232	0	4685	2.95	7.92	1.58	2.99
56	1425	1351	673	1225	0	4674	2.94	8.19	1.58	2.99
57	1431	1349	670	1227	0	4677	2.93	7.91	1.56	2.99
58	1426	1351	682	1238	0	4697	2.96	8.84	1.6	2.99
59	1429	1346	680	1226	0	4681	2.93	7.92	1.57	2.99
60	1422	1346	673	1215	0	4656	2.94	8.33	1.56	2.99

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 ⓘ



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

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, 215(IR:111, SQ:35, MR:15, LR:54, 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	%
4	3	3	4	0	14	1	1.7
1	5	1	3	0	10	2	3.3
2	1	1	2	0	6	3	5.0
2	3	0	3	0	8	4	6.7
1	2	2	3	0	8	5	8.3
1	1	0	1	0	3	6	10.0
1	2	0	0	0	3	7	11.7
2	0	0	3	0	5	8	13.3
1	3	1	0	0	5	9	15.0
1	1	1	0	0	3	10	16.7
1	2	0	0	0	3	11	18.3
1	2	2	1	0	6	12	20.0
2	3	0	2	0	7	13	21.7
1	1	0	3	0	5	14	23.3
2	3	0	2	0	7	15	25.0
0	1	1	3	0	5	16	26.7
2	0	0	0	0	2	17	28.3
2	1	0	3	0	6	18	30.0
1	2	1	3	0	7	19	31.7
9	5	3	7	0	24	20	33.3
1	2	1	2	0	6	21	35.0
0	0	0	4	0	4	22	36.7
2	0	0	5	0	7	23	38.3
2	3	0	1	0	6	24	40.0
1	2	2	3	0	8	25	41.7
0	1	0	2	0	3	26	43.3
2	0	0	2	0	4	27	45.0
2	2	0	3	0	7	28	46.7
1	1	1	1	0	4	29	48.3
2	1	3	3	0	9	30	50.0
1	2	1	2	0	6	31	51.7
0	0	3	3	0	6	32	53.3
2	1	0	1	0	4	33	55.0
1	3	2	1	0	7	34	56.7
1	1	0	3	0	5	35	58.3
1	2	3	2	0	8	36	60.0

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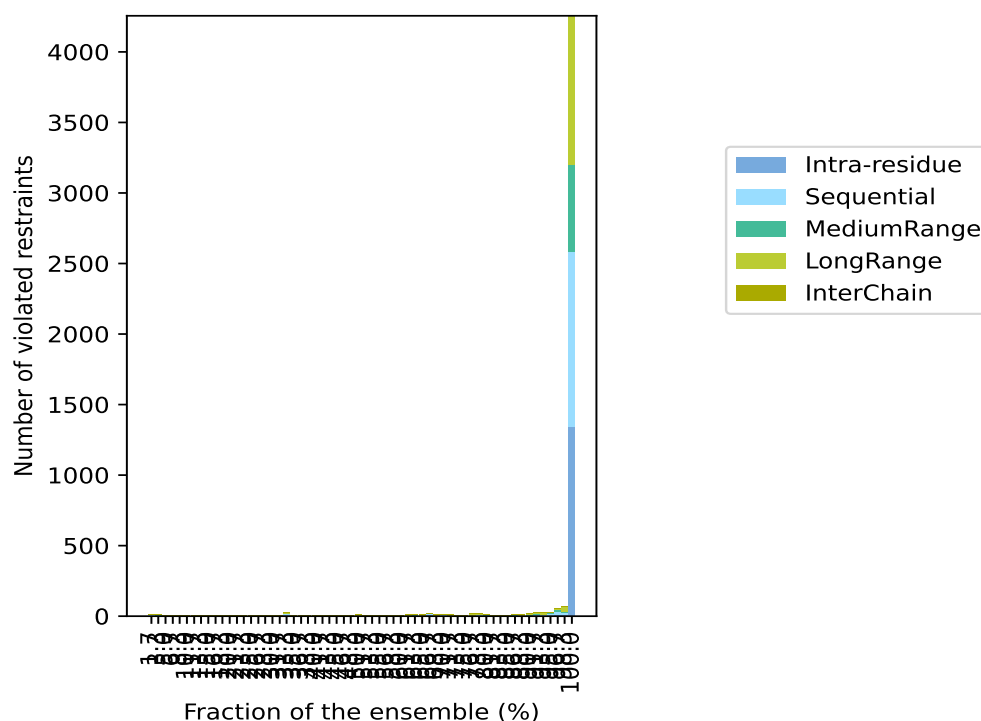
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
2	0	1	6	0	9	37	61.7
2	1	4	3	0	10	38	63.3
2	0	1	8	0	11	39	65.0
11	5	1	4	0	21	40	66.7
1	3	3	2	0	9	41	68.3
3	6	1	4	0	14	42	70.0
2	2	1	4	0	9	43	71.7
2	2	0	2	0	6	44	73.3
1	4	0	3	0	8	45	75.0
3	1	2	11	0	17	46	76.7
8	0	5	8	0	21	47	78.3
2	2	3	7	0	14	48	80.0
0	0	0	2	0	2	49	81.7
2	2	0	4	0	8	50	83.3
1	3	0	4	0	8	51	85.0
0	4	6	3	0	13	52	86.7
3	2	2	8	0	15	53	88.3
3	3	3	9	0	18	54	90.0
9	3	6	11	0	29	55	91.7
3	4	3	14	0	24	56	93.3
4	16	2	7	0	29	57	95.0
11	22	8	14	0	55	58	96.7
11	15	7	34	0	67	59	98.3
1340	1244	617	1055	0	4256	60	100.0

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

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

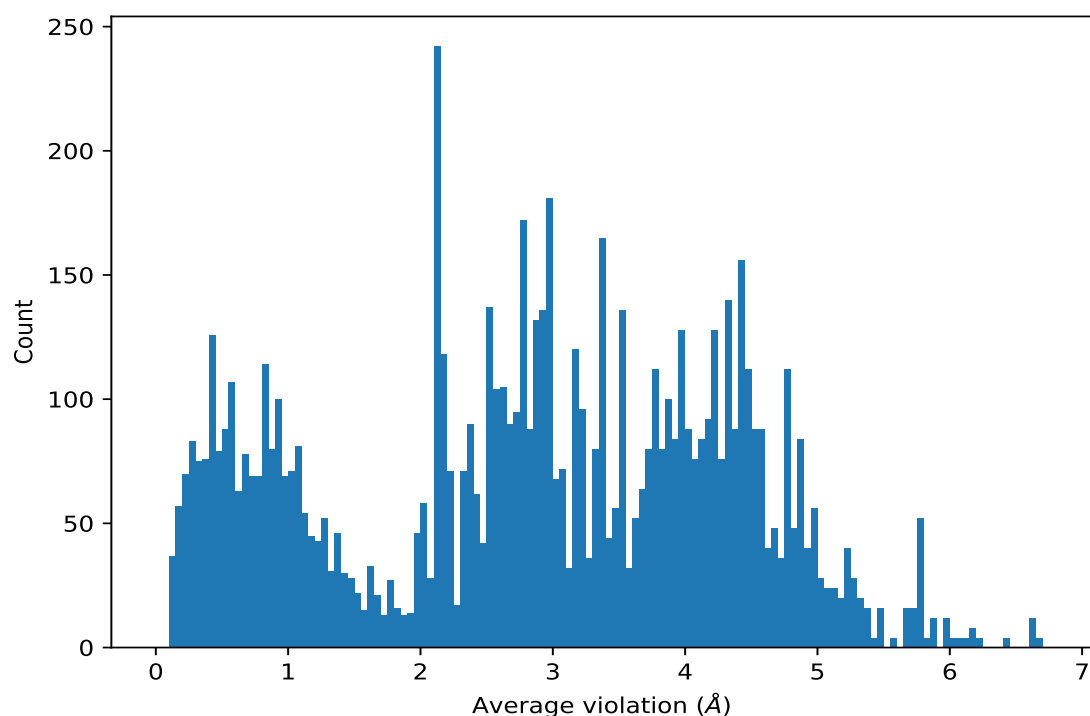
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,1568)	1:18:A:THR:H	1:19:A:LYS:HG3	60	6.68	1.5	7.72
(1,1569)	1:18:A:THR:H	1:19:A:LYS:HG3	60	6.68	1.5	7.72
(1,4167)	1:18:A:THR:H	1:19:A:LYS:HG3	60	6.68	1.5	7.72
(1,4168)	1:18:A:THR:H	1:19:A:LYS:HG3	60	6.68	1.5	7.72
(1,1630)	1:43:A:TRP:H	1:54:A:VAL:HG11	60	6.61	0.7	6.95
(1,1630)	1:43:A:TRP:H	1:54:A:VAL:HG12	60	6.61	0.7	6.95
(1,1630)	1:43:A:TRP:H	1:54:A:VAL:HG13	60	6.61	0.7	6.95
(1,1631)	1:43:A:TRP:H	1:54:A:VAL:HG11	60	6.61	0.7	6.95
(1,1631)	1:43:A:TRP:H	1:54:A:VAL:HG12	60	6.61	0.7	6.95
(1,1631)	1:43:A:TRP:H	1:54:A:VAL:HG13	60	6.61	0.7	6.95
(1,4230)	1:43:A:TRP:H	1:54:A:VAL:HG11	60	6.61	0.7	6.95
(1,4230)	1:43:A:TRP:H	1:54:A:VAL:HG12	60	6.61	0.7	6.95
(1,4230)	1:43:A:TRP:H	1:54:A:VAL:HG13	60	6.61	0.7	6.95
(1,4231)	1:43:A:TRP:H	1:54:A:VAL:HG11	60	6.61	0.7	6.95
(1,4231)	1:43:A:TRP:H	1:54:A:VAL:HG12	60	6.61	0.7	6.95
(1,4231)	1:43:A:TRP:H	1:54:A:VAL:HG13	60	6.61	0.7	6.95

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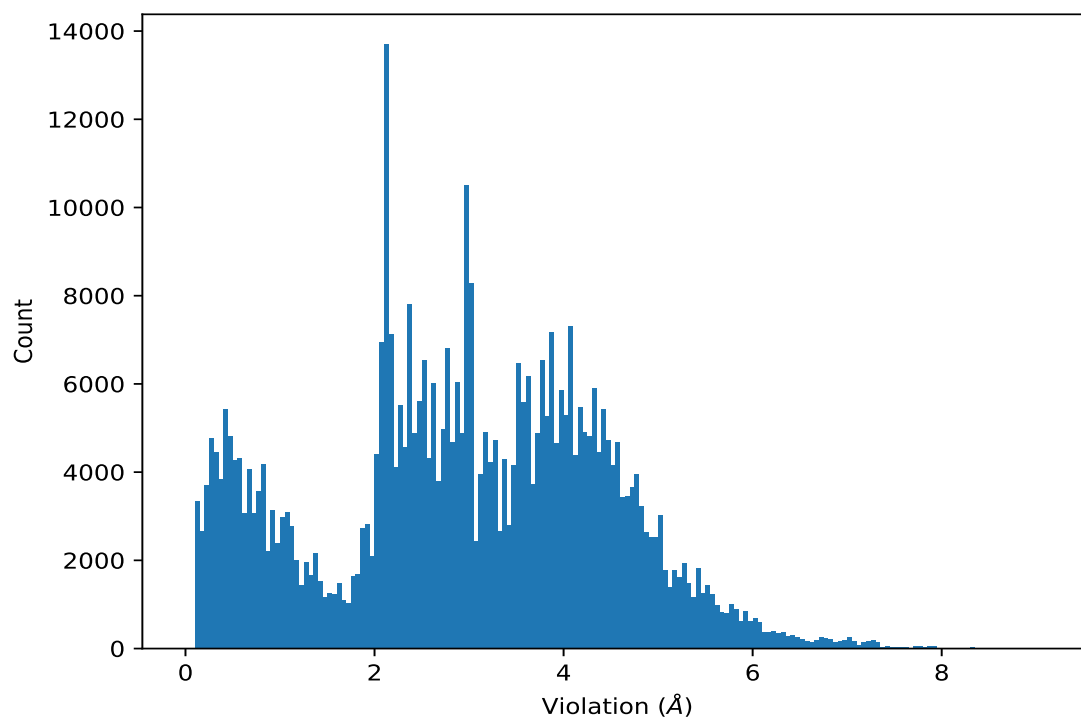
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1508)	1:46:A:ASP:HB2	1:50:A:LYS:H	60	6.4	0.62	6.14
(1,1509)	1:46:A:ASP:HB2	1:50:A:LYS:H	60	6.4	0.62	6.14

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4783)	1:46:A:ASP:HB2	1:51:A:THR:HB	17	9.15
(1,4782)	1:46:A:ASP:HB2	1:51:A:THR:HB	17	9.15
(1,2179)	1:46:A:ASP:HB2	1:51:A:THR:HB	17	9.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2178)	1:46:A:ASP:HB2	1:51:A:THR:HB	17	9.15
(1,3502)	1:33:A:TYR:HA	1:37:A:ASN:HD22	50	8.94
(1,3501)	1:33:A:TYR:HA	1:37:A:ASN:HD22	50	8.94
(1,3319)	1:34:A:ALA:H	1:37:A:ASN:HD21	13	8.94
(1,3319)	1:34:A:ALA:H	1:37:A:ASN:HD21	19	8.94
(1,3318)	1:34:A:ALA:H	1:37:A:ASN:HD21	13	8.94
(1,3318)	1:34:A:ALA:H	1:37:A:ASN:HD21	19	8.94

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

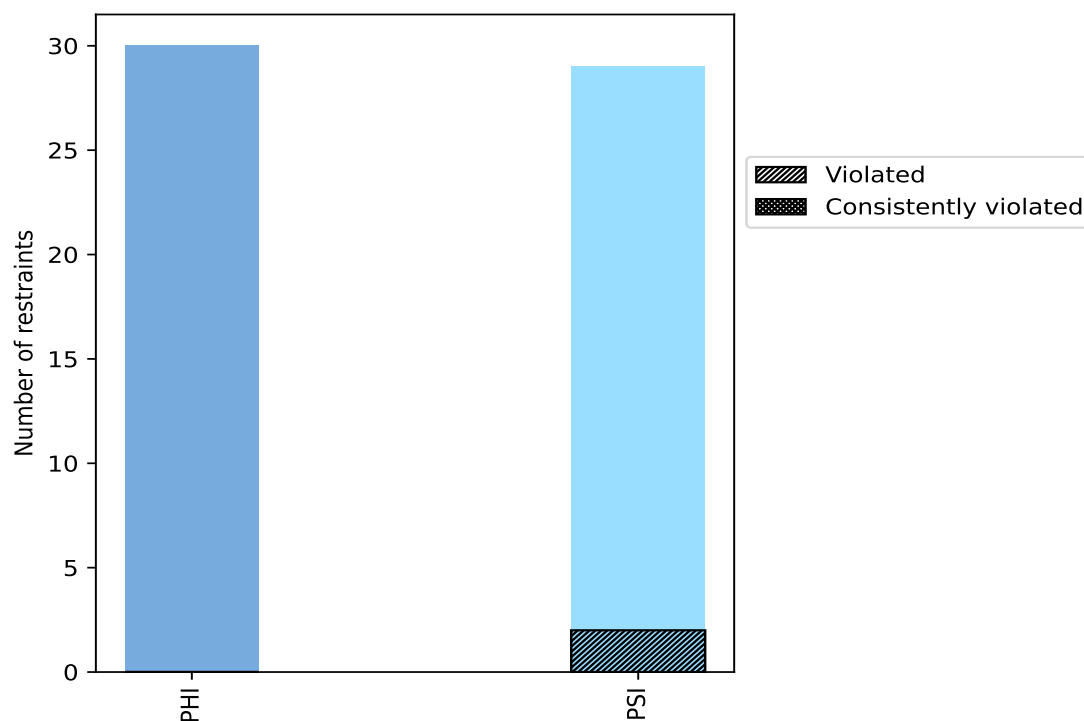
10.1 Summary of dihedral-angle violations [i](#)

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	30	50.8	0	0.0	0.0	0	0.0	0.0
PSI	29	49.2	2	6.9	3.4	0	0.0	0.0
Total	59	100.0	2	3.4	3.4	0	0.0	0.0

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

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



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

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

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

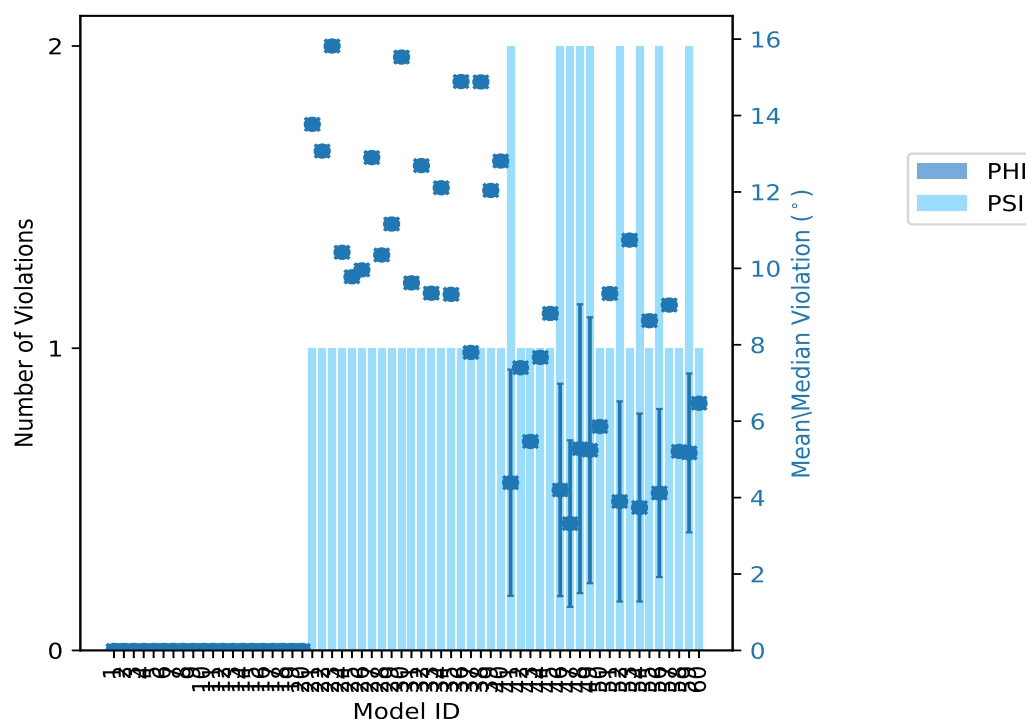
Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0.0	0.0	0.0	0.0
21	0	1	1	13.77	13.77	0.0	13.77
22	0	1	1	13.07	13.07	0.0	13.07
23	0	1	1	15.82	15.82	0.0	15.82
24	0	1	1	10.42	10.42	0.0	10.42
25	0	1	1	9.78	9.78	0.0	9.78
26	0	1	1	9.96	9.96	0.0	9.96
27	0	1	1	12.9	12.9	0.0	12.9
28	0	1	1	10.35	10.35	0.0	10.35
29	0	1	1	11.16	11.16	0.0	11.16
30	0	1	1	15.53	15.53	0.0	15.53
31	0	1	1	9.62	9.62	0.0	9.62
32	0	1	1	12.69	12.69	0.0	12.69
33	0	1	1	9.35	9.35	0.0	9.35
34	0	1	1	12.11	12.11	0.0	12.11
35	0	1	1	9.32	9.32	0.0	9.32
36	0	1	1	14.89	14.89	0.0	14.89
37	0	1	1	7.8	7.8	0.0	7.8
38	0	1	1	14.88	14.88	0.0	14.88

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Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
39	0	1	1	12.04	12.04	0.0	12.04
40	0	1	1	12.81	12.81	0.0	12.81
41	0	2	2	4.39	7.35	2.96	4.39
42	0	1	1	7.4	7.4	0.0	7.4
43	0	1	1	5.47	5.47	0.0	5.47
44	0	1	1	7.67	7.67	0.0	7.67
45	0	1	1	8.82	8.82	0.0	8.82
46	0	2	2	4.2	6.98	2.78	4.2
47	0	2	2	3.32	5.5	2.18	3.32
48	0	2	2	5.28	9.07	3.78	5.28
49	0	2	2	5.24	8.72	3.48	5.24
50	0	1	1	5.86	5.86	0.0	5.86
51	0	1	1	9.34	9.34	0.0	9.34
52	0	2	2	3.9	6.52	2.62	3.9
53	0	1	1	10.74	10.74	0.0	10.74
54	0	2	2	3.74	6.2	2.46	3.74
55	0	1	1	8.63	8.63	0.0	8.63
56	0	2	2	4.12	6.32	2.2	4.12
57	0	1	1	9.04	9.04	0.0	9.04
58	0	1	1	5.21	5.21	0.0	5.21
59	0	2	2	5.17	7.25	2.08	5.17
60	0	1	1	6.47	6.47	0.0	6.47

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	%
0	0	0	1	1.7
0	0	0	2	3.3
0	0	0	3	5.0
0	0	0	4	6.7
0	0	0	5	8.3
0	0	0	6	10.0
0	0	0	7	11.7
0	0	0	8	13.3
0	1	1	9	15.0
0	0	0	10	16.7
0	0	0	11	18.3

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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	20.0
0	0	0	13	21.7
0	0	0	14	23.3
0	0	0	15	25.0
0	0	0	16	26.7
0	0	0	17	28.3
0	0	0	18	30.0
0	0	0	19	31.7
0	0	0	20	33.3
0	0	0	21	35.0
0	0	0	22	36.7
0	0	0	23	38.3
0	0	0	24	40.0
0	0	0	25	41.7
0	0	0	26	43.3
0	0	0	27	45.0
0	0	0	28	46.7
0	0	0	29	48.3
0	0	0	30	50.0
0	0	0	31	51.7
0	0	0	32	53.3
0	0	0	33	55.0
0	0	0	34	56.7
0	0	0	35	58.3
0	0	0	36	60.0
0	0	0	37	61.7
0	0	0	38	63.3
0	0	0	39	65.0
0	1	1	40	66.7
0	0	0	41	68.3
0	0	0	42	70.0
0	0	0	43	71.7
0	0	0	44	73.3
0	0	0	45	75.0
0	0	0	46	76.7
0	0	0	47	78.3
0	0	0	48	80.0
0	0	0	49	81.7
0	0	0	50	83.3
0	0	0	51	85.0
0	0	0	52	86.7

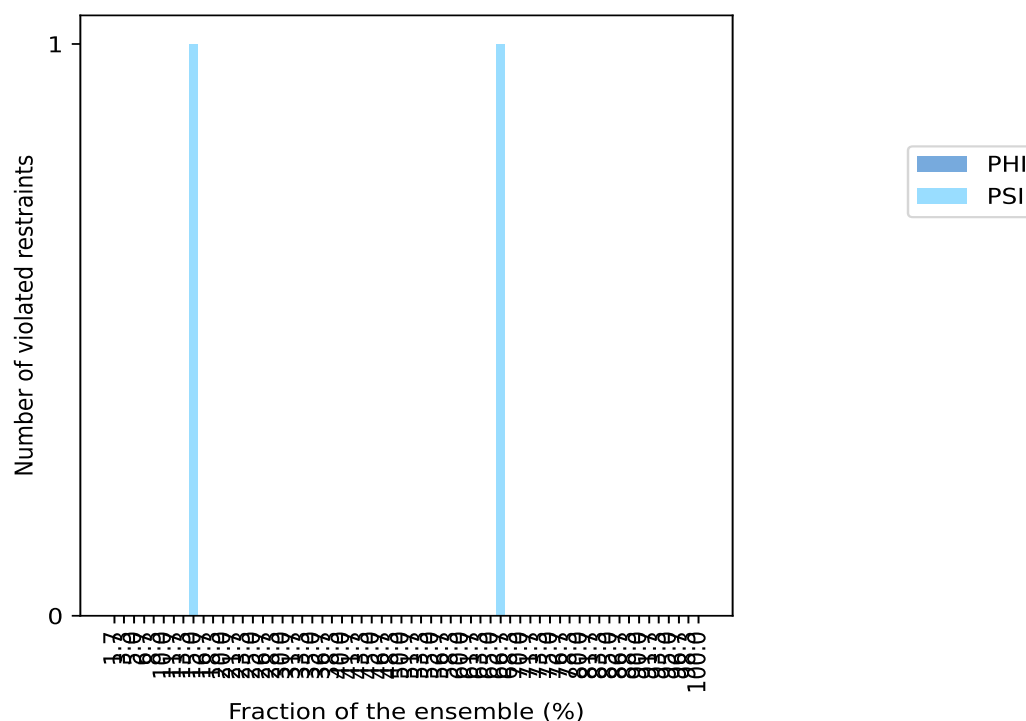
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	53	88.3
0	0	0	54	90.0
0	0	0	55	91.7
0	0	0	56	93.3
0	0	0	57	95.0
0	0	0	58	96.7
0	0	0	59	98.3
0	0	0	60	100.0

¹ Number of models with violations

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

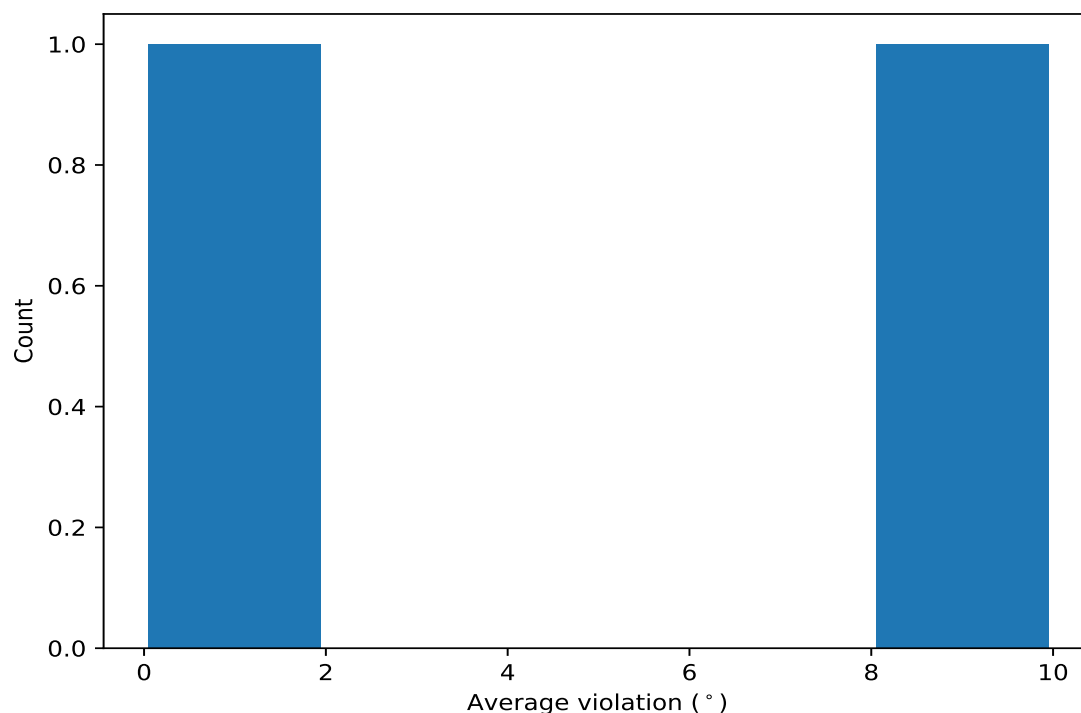


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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.

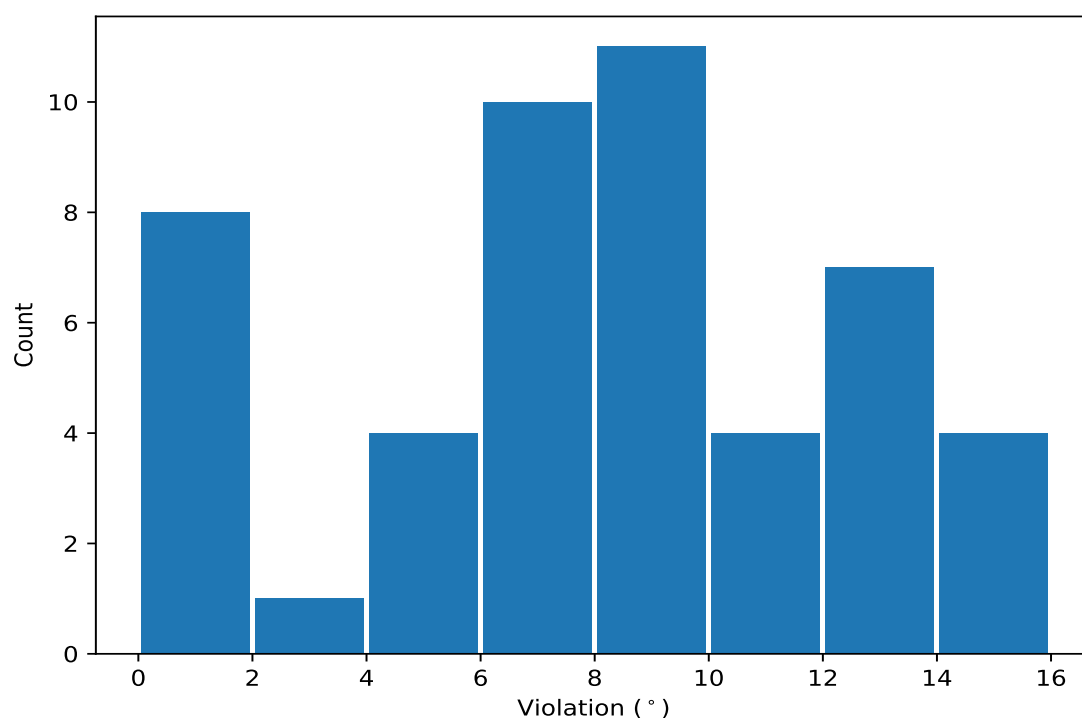
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,50)	1:49:A:THR:N	1:49:A:THR:CA	1:49:A:THR:C	1:50:A:LYS:N	40	9.67	2.95	9.33
(1,46)	1:47:A:ASP:N	1:47:A:ASP:CA	1:47:A:ASP:C	1:48:A:ALA:N	9	1.65	0.56	1.43

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 (°)
(1,50)	1:49:A:THR:N	1:49:A:THR:CA	1:49:A:THR:C	1:50:A:LYS:N	23	15.82
(1,50)	1:49:A:THR:N	1:49:A:THR:CA	1:49:A:THR:C	1:50:A:LYS:N	30	15.53
(1,50)	1:49:A:THR:N	1:49:A:THR:CA	1:49:A:THR:C	1:50:A:LYS:N	36	14.89
(1,50)	1:49:A:THR:N	1:49:A:THR:CA	1:49:A:THR:C	1:50:A:LYS:N	38	14.88
(1,50)	1:49:A:THR:N	1:49:A:THR:CA	1:49:A:THR:C	1:50:A:LYS:N	21	13.77
(1,50)	1:49:A:THR:N	1:49:A:THR:CA	1:49:A:THR:C	1:50:A:LYS:N	22	13.07
(1,50)	1:49:A:THR:N	1:49:A:THR:CA	1:49:A:THR:C	1:50:A:LYS:N	27	12.9
(1,50)	1:49:A:THR:N	1:49:A:THR:CA	1:49:A:THR:C	1:50:A:LYS:N	40	12.81
(1,50)	1:49:A:THR:N	1:49:A:THR:CA	1:49:A:THR:C	1:50:A:LYS:N	32	12.69
(1,50)	1:49:A:THR:N	1:49:A:THR:CA	1:49:A:THR:C	1:50:A:LYS:N	34	12.11