



wwPDB NMR Structure Validation Summary Report ⓘ

Jun 5, 2023 – 02:37 AM EDT

PDB ID : 2LUM
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.

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A user guide is available at

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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

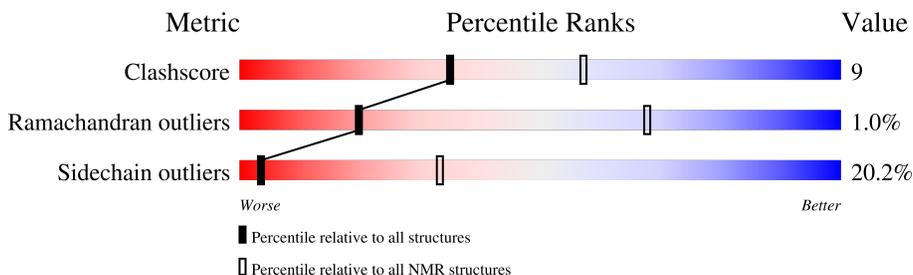
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 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	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	56	 75% 23% .

2 Ensemble composition and analysis i

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 [i](#)

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
			Total	C	H	N	O	S	
1	A	56	859	274	423	69	92	1	0

There are 2 discrepancies between the modelled and reference sequences:

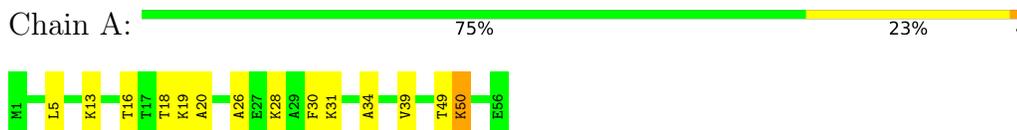
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P19909
A	2	GLN	-	expression tag	UNP P19909

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.

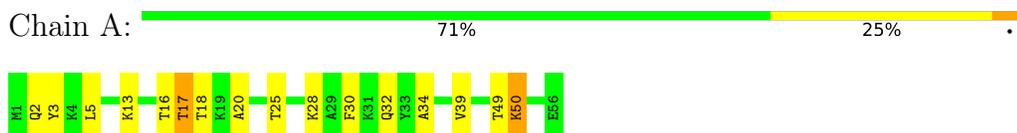
- Molecule 1: Immunoglobulin G-binding protein G



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	7±3
All	All	26160	25380	25500	449

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 87 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:20:ALA:CB	1:A:26:ALA:HB2	0.65	2.22	4	25

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%)	20	68
All	All	3240/3360 (96%)	2965 (92%)	243 (8%)	32 (1%)	20	68

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 [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	46/46 (100%)	37±2 (80±5%)	9±2 (20±5%)	3	33
All	All	2760/2760 (100%)	2203 (80%)	557 (20%)	3	33

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	53
1	A	28	LYS	39
1	A	19	LYS	34
1	A	47	ASP	30
1	A	1	MET	30

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 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	-0.21 ± 0.34	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	52	0.09 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	54	-0.16 ± 0.44	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](#)

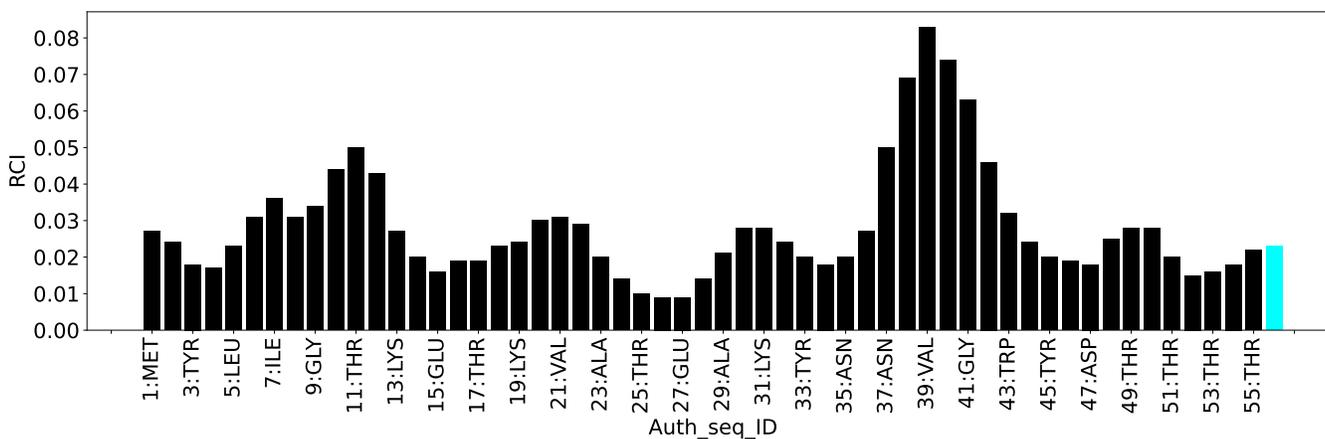
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

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	5449
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	330
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	3744
Number of restraints per residue	97.3
Number of long range restraints per residue ¹	24.3

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)	76.2	0.2
0.2-0.5 (Medium)	350.9	0.5
>0.5 (Large)	839.0	6.24

8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis

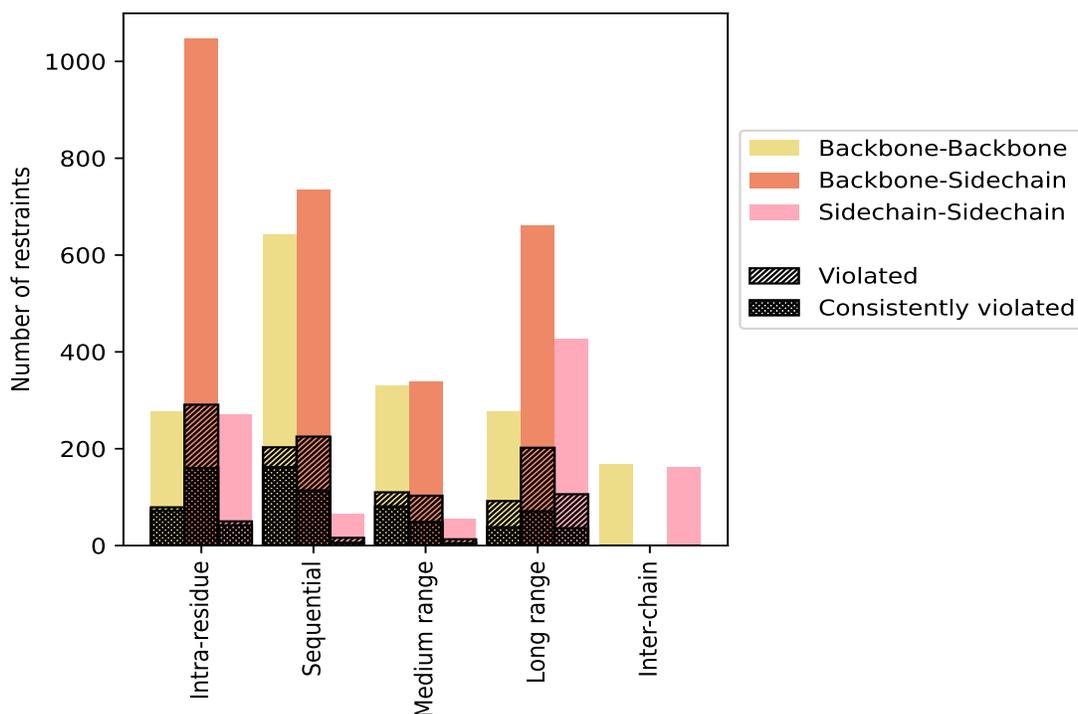
9.1 Summary of distance violations

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	29.2	420	26.4	7.7	274	17.2	5.0
Backbone-Backbone	276	5.1	79	28.6	1.4	72	26.1	1.3
Backbone-Sidechain	1047	19.2	291	27.8	5.3	160	15.3	2.9
Sidechain-Sidechain	270	5.0	50	18.5	0.9	42	15.6	0.8
Sequential ($i-j =1$)	1441	26.4	444	30.8	8.1	282	19.6	5.2
Backbone-Backbone	642	11.8	203	31.6	3.7	162	25.2	3.0
Backbone-Sidechain	734	13.5	225	30.7	4.1	114	15.5	2.1
Sidechain-Sidechain	65	1.2	16	24.6	0.3	6	9.2	0.1
Medium range ($i-j >1$ & $i-j <5$)	723	13.3	226	31.3	4.1	135	18.7	2.5
Backbone-Backbone	330	6.1	110	33.3	2.0	81	24.5	1.5
Backbone-Sidechain	339	6.2	103	30.4	1.9	49	14.5	0.9
Sidechain-Sidechain	54	1.0	13	24.1	0.2	5	9.3	0.1
Long range ($i-j \geq 5$)	1362	25.0	400	29.4	7.3	145	10.6	2.7
Backbone-Backbone	276	5.1	92	33.3	1.7	38	13.8	0.7
Backbone-Sidechain	660	12.1	202	30.6	3.7	71	10.8	1.3
Sidechain-Sidechain	426	7.8	106	24.9	1.9	36	8.5	0.7
Inter-chain	330	6.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	168	3.1	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	162	3.0	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	5449	100.0	1490	27.3	27.3	836	15.3	15.3
Backbone-Backbone	1692	31.1	484	28.6	8.9	353	20.9	6.5
Backbone-Sidechain	2780	51.0	821	29.5	15.1	394	14.2	7.2
Sidechain-Sidechain	977	17.9	185	18.9	3.4	89	9.1	1.6

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	363	383	202	315	0	1263	0.91	5.41	0.7	0.74
2	361	389	196	318	0	1264	0.9	5.17	0.68	0.74
3	366	382	204	320	0	1272	0.92	5.19	0.7	0.74
4	359	383	197	315	0	1254	0.91	5.04	0.67	0.74
5	352	382	204	303	0	1241	0.97	5.07	0.75	0.77
6	352	383	203	321	0	1259	0.94	5.78	0.75	0.74
7	361	385	195	316	0	1257	0.92	5.35	0.72	0.72
8	358	387	197	312	0	1254	0.89	5.67	0.66	0.72
9	365	374	195	316	0	1250	0.9	5.06	0.67	0.73
10	354	373	197	309	0	1233	0.91	4.83	0.69	0.74
11	368	381	202	315	0	1266	0.94	4.99	0.75	0.74

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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	361	384	203	322	0	1270	0.95	5.09	0.74	0.76
13	362	379	195	317	0	1253	0.91	5.41	0.7	0.73
14	360	389	197	326	0	1272	0.93	4.79	0.71	0.74
15	357	378	198	307	0	1240	0.9	5.1	0.66	0.73
16	371	384	202	309	0	1266	0.89	5.01	0.67	0.72
17	354	387	203	322	0	1266	0.93	6.24	0.76	0.72
18	361	390	198	299	0	1248	0.89	4.65	0.66	0.73
19	361	383	197	306	0	1247	0.92	5.82	0.74	0.73
20	362	378	201	336	0	1277	0.96	5.7	0.75	0.76
21	364	388	195	325	0	1272	0.86	3.81	0.59	0.71
22	369	392	194	325	0	1280	0.85	3.86	0.6	0.69
23	363	389	187	317	0	1256	0.88	5.06	0.65	0.73
24	368	390	196	319	0	1273	0.94	5.08	0.76	0.73
25	369	389	195	327	0	1280	0.86	4.47	0.61	0.7
26	378	389	195	316	0	1278	0.86	4.42	0.62	0.69
27	367	392	192	319	0	1270	0.85	4.88	0.63	0.67
28	371	391	196	318	0	1276	0.86	4.48	0.61	0.71
29	361	392	196	314	0	1263	0.91	5.18	0.7	0.74
30	369	394	191	313	0	1267	0.86	4.45	0.62	0.72
31	371	390	190	326	0	1277	0.9	4.85	0.69	0.73
32	372	394	193	320	0	1279	0.87	4.48	0.62	0.7
33	370	383	195	320	0	1268	0.94	5.29	0.72	0.74
34	368	384	193	319	0	1264	0.91	5.0	0.73	0.73
35	370	392	198	325	0	1285	0.94	5.07	0.75	0.74
36	367	387	190	325	0	1269	0.89	3.78	0.62	0.73
37	362	385	193	317	0	1257	0.88	5.07	0.67	0.73
38	378	391	193	324	0	1286	0.87	4.83	0.65	0.71
39	366	395	188	329	0	1278	0.89	4.59	0.68	0.72
40	370	398	191	320	0	1279	0.85	4.35	0.61	0.69
41	369	389	196	311	0	1265	0.94	5.38	0.76	0.75
42	364	382	199	315	0	1260	0.94	4.72	0.73	0.75
43	367	392	192	320	0	1271	0.91	4.63	0.68	0.73
44	371	380	194	325	0	1270	0.92	4.72	0.69	0.74
45	367	387	194	322	0	1270	0.91	4.74	0.7	0.72
46	367	384	196	321	0	1268	0.91	4.61	0.69	0.74
47	370	387	197	332	0	1286	0.93	4.48	0.7	0.75
48	363	385	197	325	0	1270	0.92	4.74	0.71	0.74
49	372	383	192	314	0	1261	0.88	4.5	0.64	0.72
50	372	395	199	337	0	1303	1.02	5.52	0.85	0.77
51	365	387	193	318	0	1263	0.92	4.83	0.66	0.76
52	362	390	192	321	0	1265	0.9	4.76	0.68	0.75

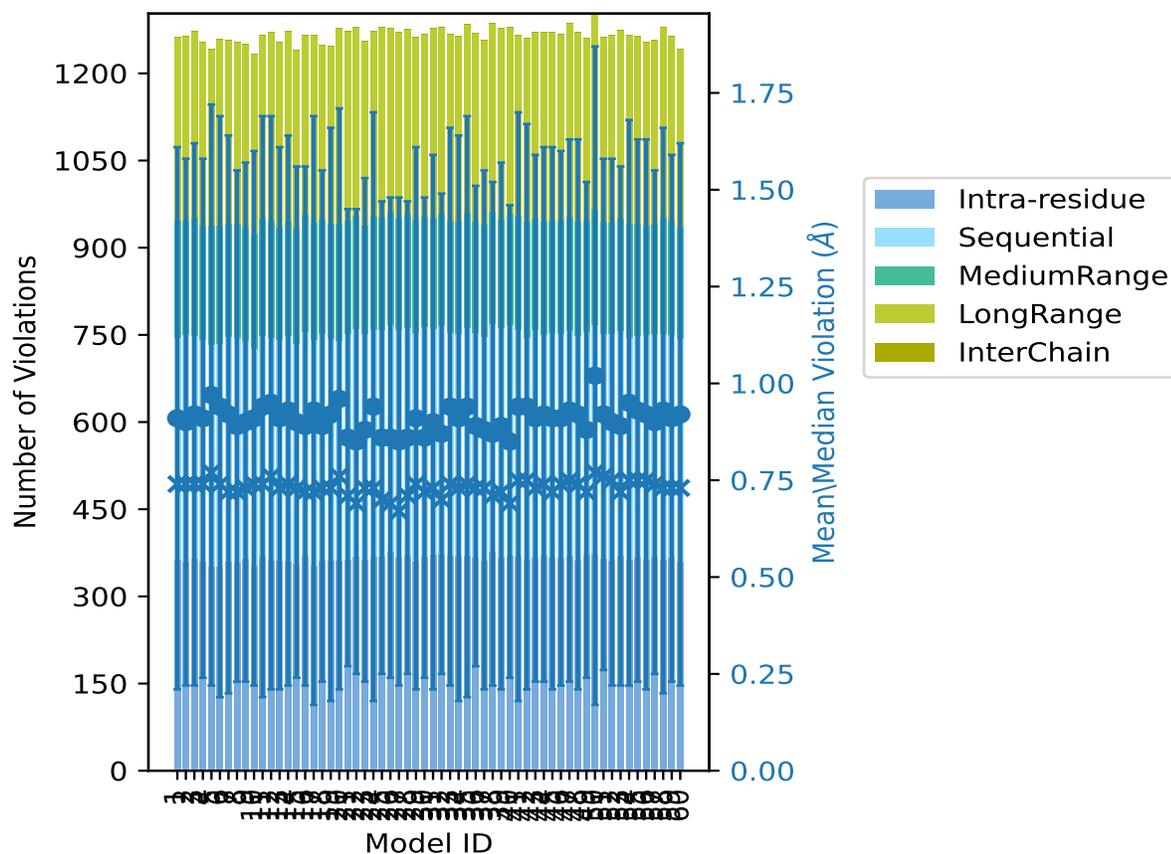
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
53	370	388	192	324	0	1274	0.89	4.48	0.67	0.72
54	364	380	198	324	0	1266	0.95	4.63	0.73	0.75
55	366	383	192	323	0	1264	0.93	4.68	0.7	0.75
56	363	387	189	315	0	1254	0.92	4.66	0.71	0.75
57	368	384	187	318	0	1257	0.9	4.72	0.65	0.74
58	364	388	200	328	0	1280	0.93	5.31	0.73	0.73
59	367	383	196	318	0	1264	0.91	4.64	0.68	0.73
60	360	384	191	307	0	1242	0.92	4.8	0.7	0.73

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, 3959(IR:1173, SQ:997, MR:497, LR:962, IC:330) 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	2	1	3	0	8	3	5.0
2	2	0	2	0	6	4	6.7
2	2	2	3	0	9	5	8.3
1	2	0	1	0	4	6	10.0
0	1	0	0	0	1	7	11.7
2	0	0	3	0	5	8	13.3
1	4	1	0	0	6	9	15.0
1	0	1	0	0	2	10	16.7
1	3	1	1	0	6	11	18.3
1	1	1	0	0	3	12	20.0
3	4	0	2	0	9	13	21.7
1	1	0	3	0	5	14	23.3
2	2	0	3	0	7	15	25.0
0	1	1	2	0	4	16	26.7
3	1	0	0	0	4	17	28.3
1	1	0	3	0	5	18	30.0
1	2	1	3	0	7	19	31.7
8	5	3	7	0	23	20	33.3
1	2	1	3	0	7	21	35.0
0	1	0	4	0	5	22	36.7
3	1	0	4	0	8	23	38.3
2	2	0	2	0	6	24	40.0
1	1	2	3	0	7	25	41.7
0	1	0	1	0	2	26	43.3
1	0	0	3	0	4	27	45.0
2	2	0	2	0	6	28	46.7
1	1	2	1	0	5	29	48.3
2	2	3	3	0	10	30	50.0
1	1	0	3	0	5	31	51.7
1	1	3	3	0	8	32	53.3
1	2	0	0	0	3	33	55.0
1	2	2	3	0	8	34	56.7
1	0	1	1	0	3	35	58.3
1	2	2	2	0	7	36	60.0

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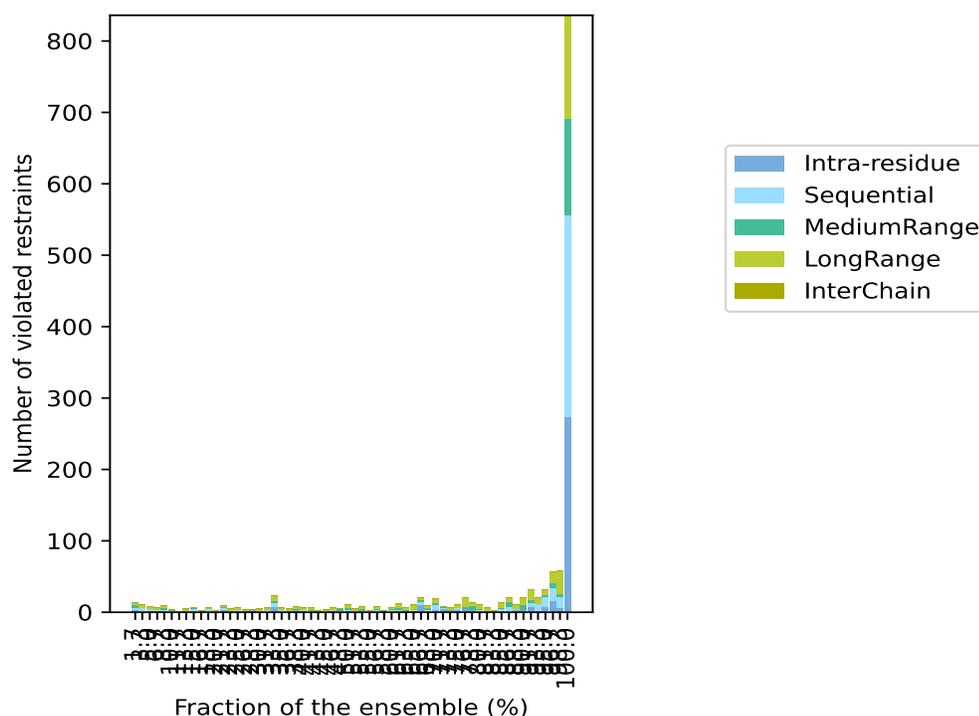
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
3	0	3	6	0	12	37	61.7
1	0	2	4	0	7	38	63.3
3	0	1	7	0	11	39	65.0
10	5	2	4	0	21	40	66.7
1	3	2	3	0	9	41	68.3
3	8	2	6	0	19	42	70.0
5	2	0	1	0	8	43	71.7
1	2	0	3	0	6	44	73.3
3	3	0	5	0	11	45	75.0
5	0	3	12	0	20	46	76.7
4	0	5	5	0	14	47	78.3
1	2	2	6	0	11	48	80.0
0	0	0	6	0	6	49	81.7
1	2	0	0	0	3	50	83.3
1	4	2	7	0	14	51	85.0
1	6	8	5	0	20	52	86.7
3	2	0	6	0	11	53	88.3
4	0	6	10	0	20	54	90.0
8	5	4	14	0	31	55	91.7
2	9	1	9	0	21	56	93.3
8	13	4	7	0	32	57	95.0
16	18	7	16	0	57	58	96.7
6	15	5	32	0	58	59	98.3
274	282	135	145	0	836	60	100.0

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

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

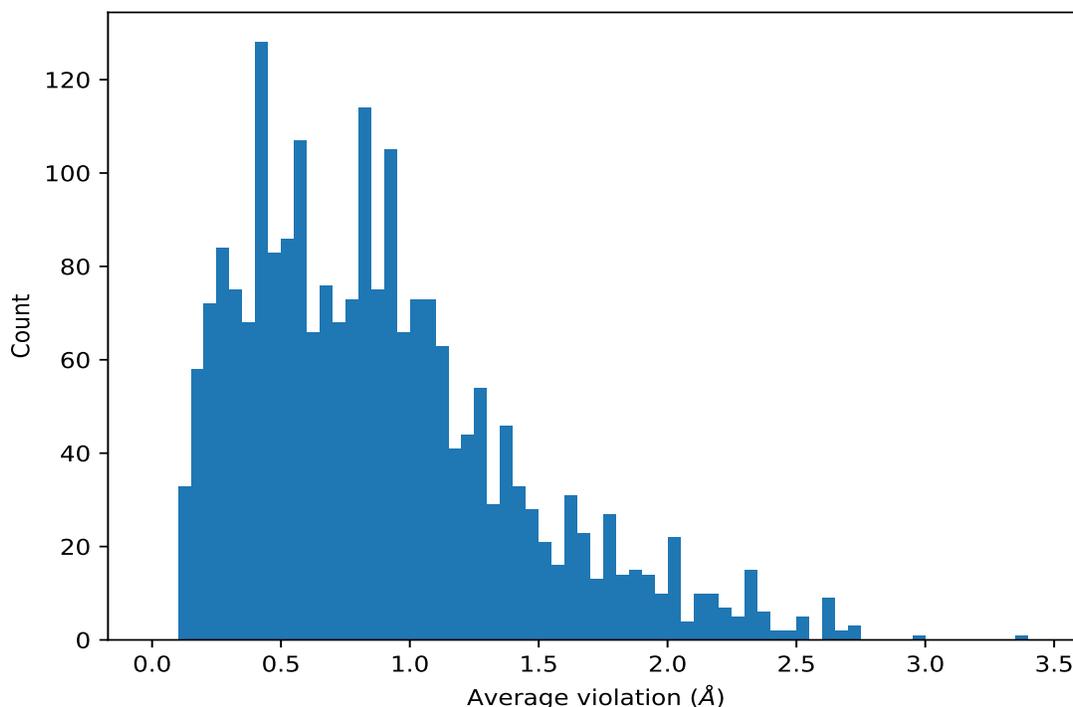
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,4166)	1:A:18:THR:H	1:A:19:LYS:HG3	60	3.4	1.5	4.44
(1,4169)	1:A:28:LYS:H	1:A:31:LYS:HG3	60	2.95	1.48	2.64
(1,4883)	1:A:15:GLU:HB3	1:A:17:THR:HG21	60	2.72	0.95	3.24
(1,4883)	1:A:15:GLU:HB3	1:A:17:THR:HG22	60	2.72	0.95	3.24
(1,4883)	1:A:15:GLU:HB3	1:A:17:THR:HG23	60	2.72	0.95	3.24
(1,4775)	1:A:43:TRP:HB3	1:A:54:VAL:HB	60	2.68	1.09	2.26
(1,4028)	1:A:5:LEU:H	1:A:15:GLU:HB2	60	2.67	0.79	3.07
(1,4757)	1:A:41:GLY:HA2	1:A:54:VAL:HG21	60	2.63	1.45	2.64
(1,4757)	1:A:41:GLY:HA2	1:A:54:VAL:HG22	60	2.63	1.45	2.64
(1,4757)	1:A:41:GLY:HA2	1:A:54:VAL:HG23	60	2.63	1.45	2.64
(1,4229)	1:A:43:TRP:H	1:A:54:VAL:HG11	60	2.6	0.7	2.94
(1,4229)	1:A:43:TRP:H	1:A:54:VAL:HG12	60	2.6	0.7	2.94
(1,4229)	1:A:43:TRP:H	1:A:54:VAL:HG13	60	2.6	0.7	2.94
(1,4145)	1:A:48:ALA:HB1	1:A:50:LYS:H	60	2.53	0.75	2.1
(1,4145)	1:A:48:ALA:HB2	1:A:50:LYS:H	60	2.53	0.75	2.1
(1,4145)	1:A:48:ALA:HB3	1:A:50:LYS:H	60	2.53	0.75	2.1

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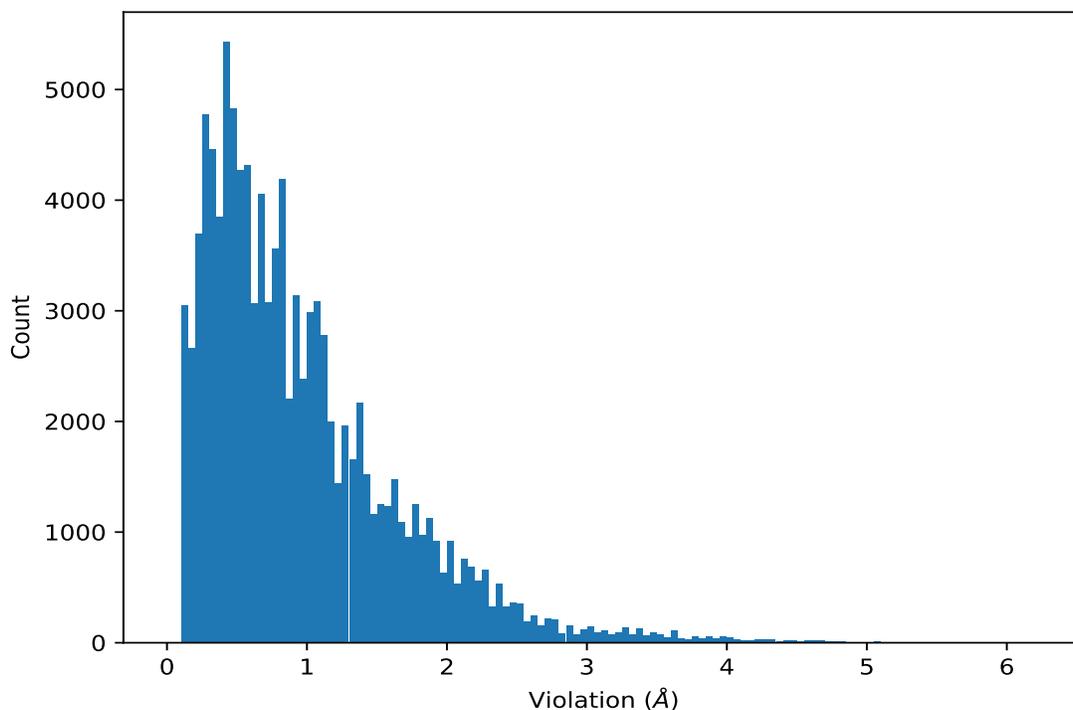
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4175)	1:A:49:THR:H	1:A:50:LYS:HG3	60	2.53	0.72	2.72
(1,4778)	1:A:2:GLN:HB2	1:A:17:THR:HB	60	2.53	1.17	2.48

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)
(1,4781)	1:A:46:ASP:HB2	1:A:51:THR:HB	17	6.24
(1,4781)	1:A:46:ASP:HB2	1:A:51:THR:HB	19	5.82
(1,4781)	1:A:46:ASP:HB2	1:A:51:THR:HB	6	5.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4781)	1:A:46:ASP:HB2	1:A:51:THR:HB	20	5.7
(1,4781)	1:A:46:ASP:HB2	1:A:51:THR:HB	8	5.67
(1,898)	1:A:33:TYR:HA	1:A:37:ASN:HD21	50	5.52
(1,3497)	1:A:33:TYR:HA	1:A:37:ASN:HD21	50	5.52
(1,718)	1:A:34:ALA:H	1:A:37:ASN:HD21	13	5.41
(1,718)	1:A:34:ALA:H	1:A:37:ASN:HD21	19	5.41
(1,4169)	1:A:28:LYS:H	1:A:31:LYS:HG3	1	5.41

10 Dihedral-angle violation analysis

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value