



wwPDB NMR Structure Validation Summary Report ⓘ

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BMRB ID : 19067
Title : Solution structure of latherin
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Deposited on : 2013-02-28

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

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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 : 4-5-2 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

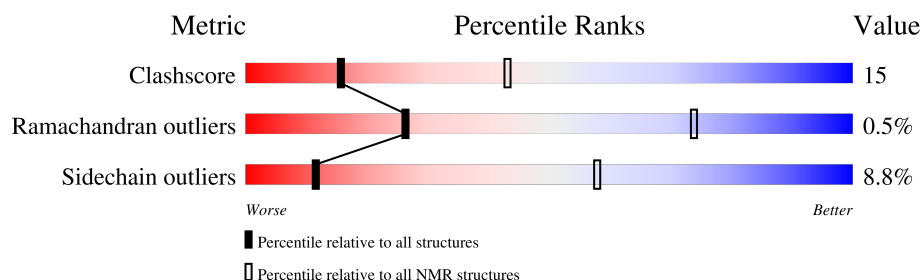
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 94%.

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	211	

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models).

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:3-A:43, A:62-A:77, A:83-A:96, A:104-A:119, A:126-A:142, A:157-A:200 (148)	0.33	8

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 and 6 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3288 atoms, of which 1677 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called LATHERIN.

Mol	Chain	Residues	Atoms						Trace
1	A	211	Total	C	H	N	O	S	0
			3288	1029	1677	264	315	3	

There are 3 discrepancies between the modelled and reference sequences:

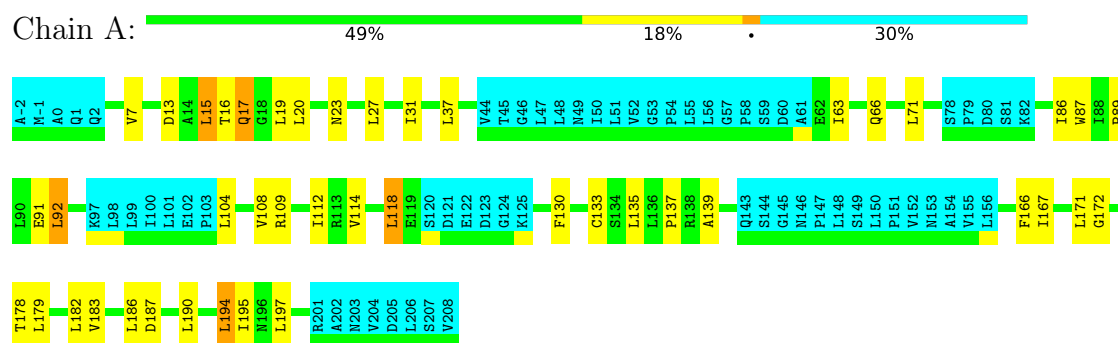
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP P82615
A	-1	MET	-	expression tag	UNP P82615
A	0	ALA	-	expression tag	UNP P82615

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: LATHERIN



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

The representative model is number 8. Colouring as in section 4.1 above.

- Molecule 1: LATHERIN



5 Refinement protocol and experimental data overview

The models were refined using the following method: *AS PER PUBLICATION*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
CNS	refinement	
CcpNmr Analysis	structure solution	2.1
CcpNmr Analysis	structure solution	2.2
CcpNmr Analysis	structure solution	2.0
DANGLE	structure solution	1.1
TopSpin	structure solution	1.3
CNS	structure solution	1.2

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2652
Number of shifts mapped to atoms	2652
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

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	0.57±0.01	0±0/1172 (0.0± 0.0%)	0.77±0.02	0±0/1601 (0.0± 0.0%)
All	All	0.57	0/23440 (0.0%)	0.77	1/32020 (0.0%)

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	71	LEU	CB-CA-C	-5.07	109.77	117.07	11	1

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	1157	1202	1201	34±3
All	All	23140	24040	24020	689

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 15.

5 of 142 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:ARG:HB3	1:A:139:ALA:HB3	0.81	1.53	12	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:THR:HA	1:A:19:LEU:HD12	0.79	1.55	1	19
1:A:16:THR:O	1:A:20:LEU:HG	0.74	1.82	7	20
1:A:108:VAL:HG21	1:A:167:ILE:HD11	0.74	1.58	20	20
1:A:16:THR:HA	1:A:19:LEU:HD22	0.73	1.60	13	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	148/211 (70%)	136±2 (92±1%)	11±2 (7±1%)	1±1 (1±1%)	26	74
All	All	2960/4220 (70%)	2727 (92%)	217 (7%)	16 (1%)	26	74

All 5 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	23	ASN	7
1	A	32	ASN	5
1	A	22	GLY	2
1	A	178	THR	1
1	A	3	ILE	1

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	133/186 (72%)	121±2 (91±1%)	12±2 (9±1%)	11	58
All	All	2660/3720 (72%)	2427 (91%)	233 (9%)	11	58

5 of 36 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	15	LEU	20
1	A	17	GLN	20
1	A	114	VAL	20
1	A	186	LEU	20
1	A	118	LEU	18

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 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

The completeness of assignment taking into account all chemical shift lists is 94% for the well-defined parts and 91% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping

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	2652
Number of shifts mapped to atoms	2652
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	204	-0.33 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	192	0.10 ± 0.05	None needed (< 0.5 ppm)
$^{13}\text{C}'$	196	-0.07 ± 0.04	None needed (< 0.5 ppm)
^{15}N	189	0.35 ± 0.23	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 94%, i.e. 1974 atoms were assigned a chemical shift out of a possible 2096. 0 out of 43 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	736/739 (100%)	299/300 (100%)	294/296 (99%)	143/143 (100%)
Sidechain	1164/1270 (92%)	797/837 (95%)	353/396 (89%)	14/37 (38%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	74/87 (85%)	38/42 (90%)	35/42 (83%)	1/3 (33%)
Overall	1974/2096 (94%)	1134/1179 (96%)	682/734 (93%)	158/183 (86%)

7.1.4 Statistically unusual chemical shifts [i](#)

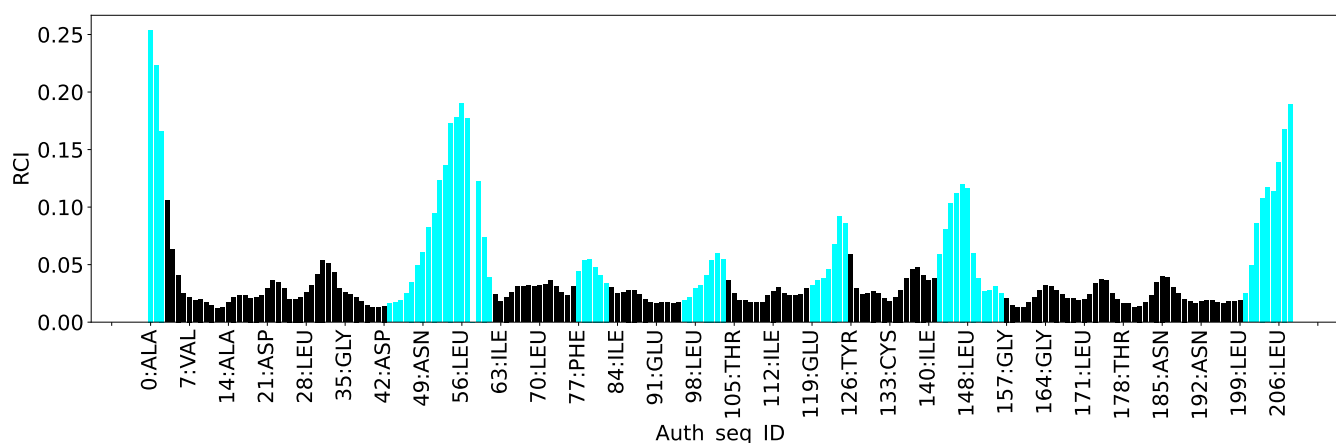
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	113	ARG	HG2	-0.27	0.26 – 2.87	-7.0

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	90442
Intra-residue ($ i-j =0$)	3587
Sequential ($ i-j =1$)	2733
Medium range ($ i-j >1$ and $ i-j <5$)	4054
Long range ($ i-j \geq 5$)	80068
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	428.6
Number of long range restraints per residue ¹	379.5

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)	620.9	0.2
0.2-0.5 (Medium)	1606.1	0.5
>0.5 (Large)	83036.9	71.71

8.2.2 Average number of dihedral-angle violations per model [i](#)

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

9 Distance violation analysis ⓘ

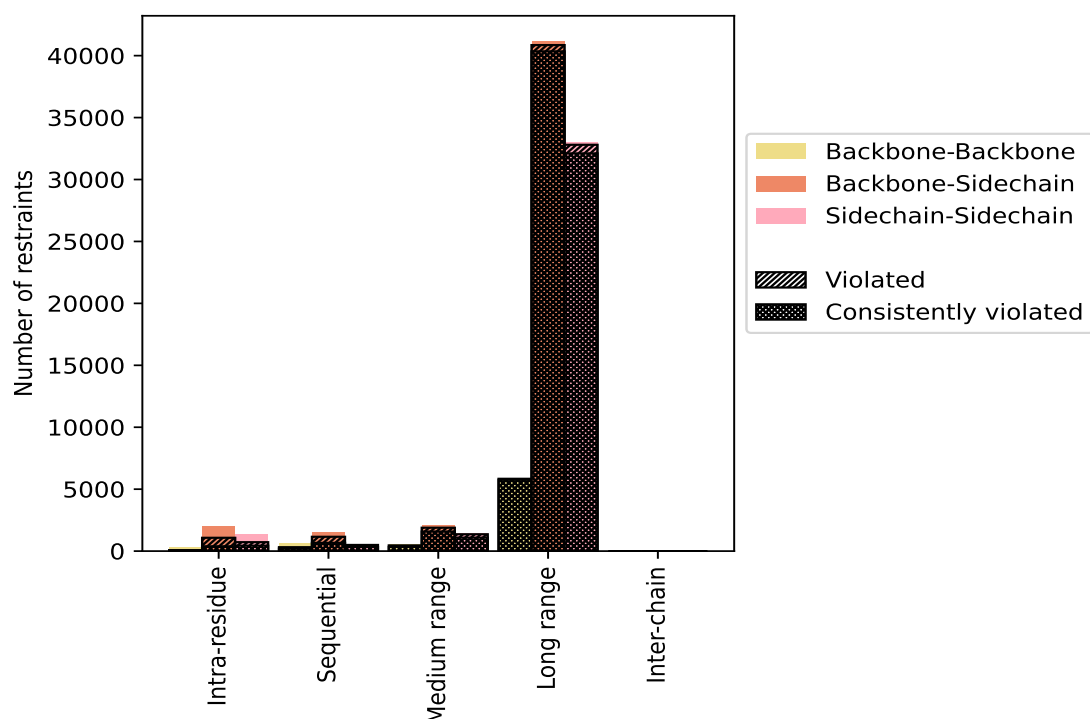
9.1 Summary of distance violations ⓘ

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)	3587	4.0	1873	52.2	2.1	878	24.5	1.0
Backbone-Backbone	294	0.3	76	25.9	0.1	52	17.7	0.1
Backbone-Sidechain	1972	2.2	1076	54.6	1.2	388	19.7	0.4
Sidechain-Sidechain	1321	1.5	721	54.6	0.8	438	33.2	0.5
Sequential (i-j =1)	2733	3.0	1970	72.1	2.2	1202	44.0	1.3
Backbone-Backbone	620	0.7	316	51.0	0.3	204	32.9	0.2
Backbone-Sidechain	1550	1.7	1157	74.6	1.3	665	42.9	0.7
Sidechain-Sidechain	563	0.6	497	88.3	0.5	333	59.1	0.4
Medium range (i-j >1 & i-j <5)	4054	4.5	3710	91.5	4.1	3001	74.0	3.3
Backbone-Backbone	580	0.6	462	79.7	0.5	337	58.1	0.4
Backbone-Sidechain	2055	2.3	1888	91.9	2.1	1577	76.7	1.7
Sidechain-Sidechain	1419	1.6	1360	95.8	1.5	1087	76.6	1.2
Long range (i-j ≥5)	80068	88.5	79496	99.3	87.9	78205	97.7	86.5
Backbone-Backbone	5896	6.5	5839	99.0	6.5	5753	97.6	6.4
Backbone-Sidechain	41159	45.5	40853	99.3	45.2	40344	98.0	44.6
Sidechain-Sidechain	33013	36.5	32804	99.4	36.3	32108	97.3	35.5
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	90442	100.0	87049	96.2	96.2	83286	92.1	92.1
Backbone-Backbone	7390	8.2	6693	90.6	7.4	6346	85.9	7.0
Backbone-Sidechain	46736	51.7	44974	96.2	49.7	42974	92.0	47.5
Sidechain-Sidechain	36316	40.2	35382	97.4	39.1	33966	93.5	37.6

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 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	1349	1617	3434	78933	0	85333	18.6	70.39	13.01	16.05
2	1342	1624	3408	78935	0	85309	18.42	63.43	12.74	16.03
3	1340	1609	3411	78953	0	85313	18.6	69.97	13.02	16.07
4	1350	1610	3416	78935	0	85311	18.43	66.16	12.8	16.01
5	1329	1609	3404	78918	0	85260	18.49	68.95	12.91	15.99
6	1319	1609	3405	78949	0	85282	18.65	71.71	13.02	16.13
7	1346	1615	3407	78954	0	85322	18.55	68.23	12.88	16.08
8	1326	1622	3411	78912	0	85271	18.38	64.97	12.67	16.0
9	1338	1601	3422	78953	0	85314	18.52	71.08	12.88	16.05
10	1340	1621	3433	78931	0	85325	18.58	70.51	12.91	16.1

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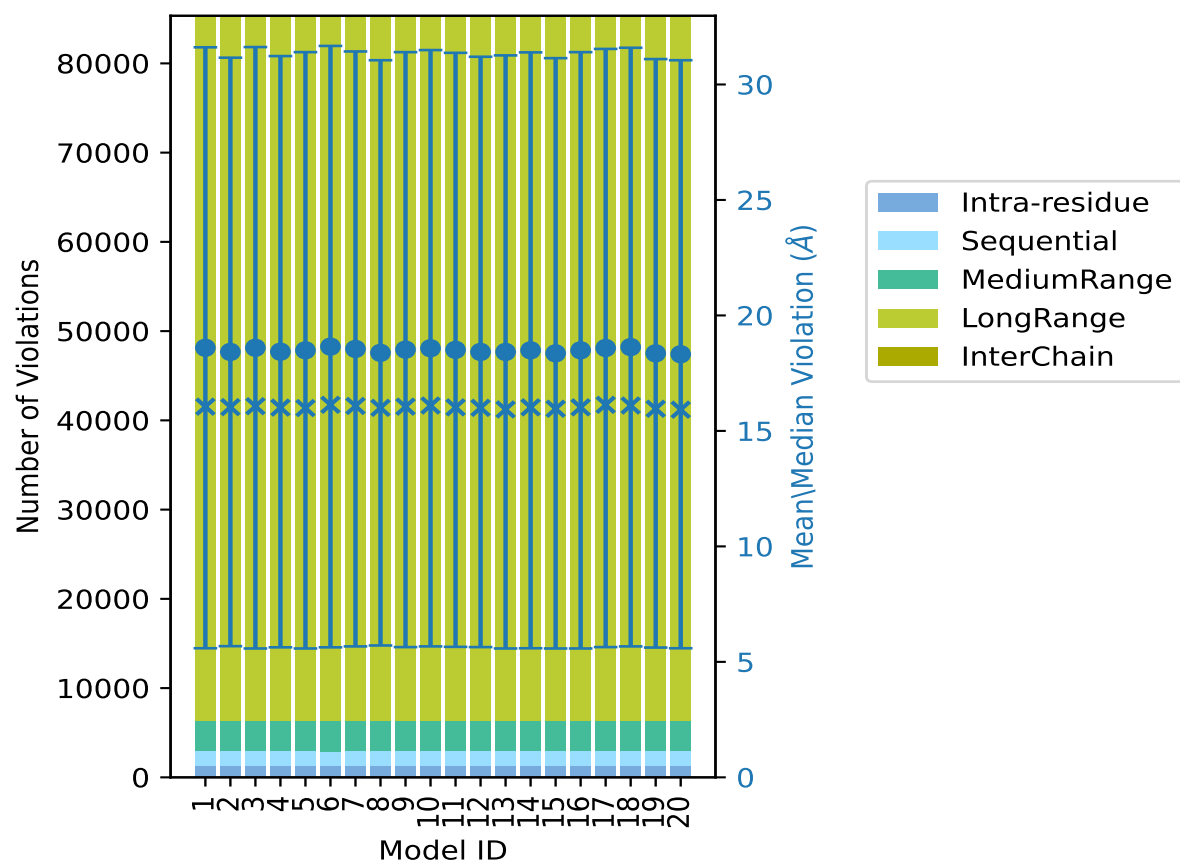
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1331	1613	3403	78956	0	85303	18.51	70.87	12.86	16.02
12	1336	1618	3385	78933	0	85272	18.42	67.79	12.78	16.0
13	1335	1615	3388	78954	0	85292	18.42	69.38	12.84	15.93
14	1344	1598	3404	78912	0	85258	18.49	68.89	12.9	16.02
15	1338	1607	3378	78939	0	85262	18.36	69.38	12.78	15.96
16	1348	1606	3421	78931	0	85306	18.49	67.67	12.91	16.02
17	1329	1606	3407	78942	0	85284	18.59	70.03	12.95	16.13
18	1324	1601	3417	78930	0	85272	18.63	67.61	12.96	16.1
19	1333	1600	3419	78940	0	85292	18.36	68.04	12.74	15.96
20	1333	1616	3408	78946	0	85303	18.32	69.16	12.73	15.92

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

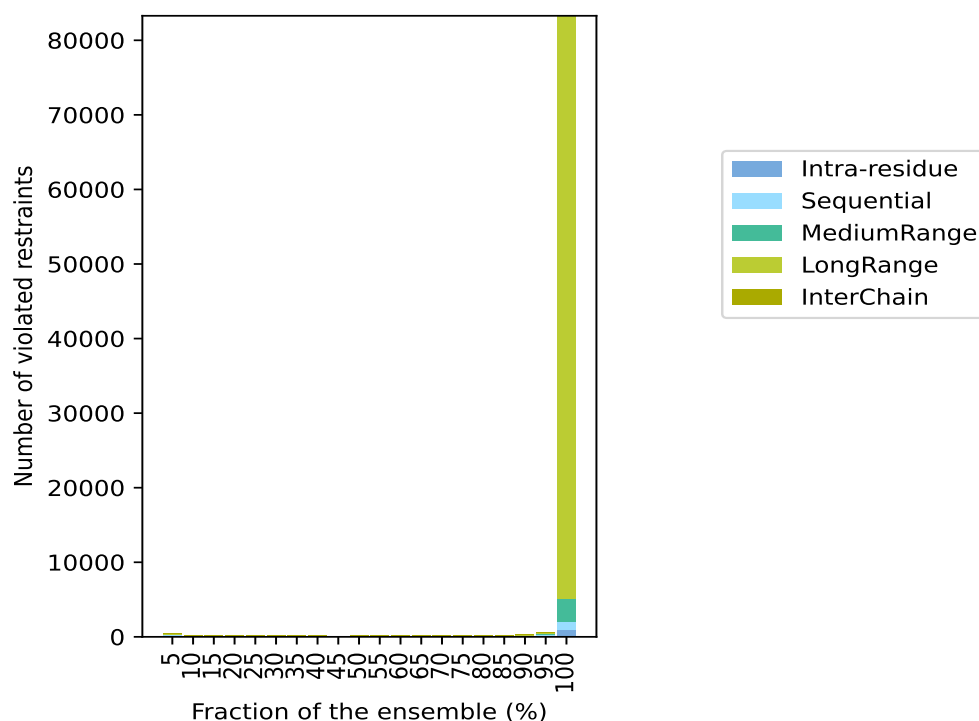
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3393(IR:1714, SQ:763, MR:344, LR:572, IC:0) restraints are 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	%
147	86	71	111	0	415	1	5.0
71	36	31	69	0	207	2	10.0
59	39	38	79	0	215	3	15.0
63	38	27	50	0	178	4	20.0
59	27	20	47	0	153	5	25.0
34	28	17	45	0	124	6	30.0
43	27	24	35	0	129	7	35.0
43	26	9	42	0	120	8	40.0
26	26	19	30	0	101	9	45.0
36	23	27	43	0	129	10	50.0
23	31	27	56	0	137	11	55.0
24	34	32	35	0	125	12	60.0
33	39	32	41	0	145	13	65.0
21	29	34	43	0	127	14	70.0
38	36	24	60	0	158	15	75.0
67	29	37	61	0	194	16	80.0
49	41	49	97	0	236	17	85.0
46	64	64	105	0	279	18	90.0
113	109	127	242	0	591	19	95.0
878	1202	3001	78205	0	83286	20	100.0

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

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

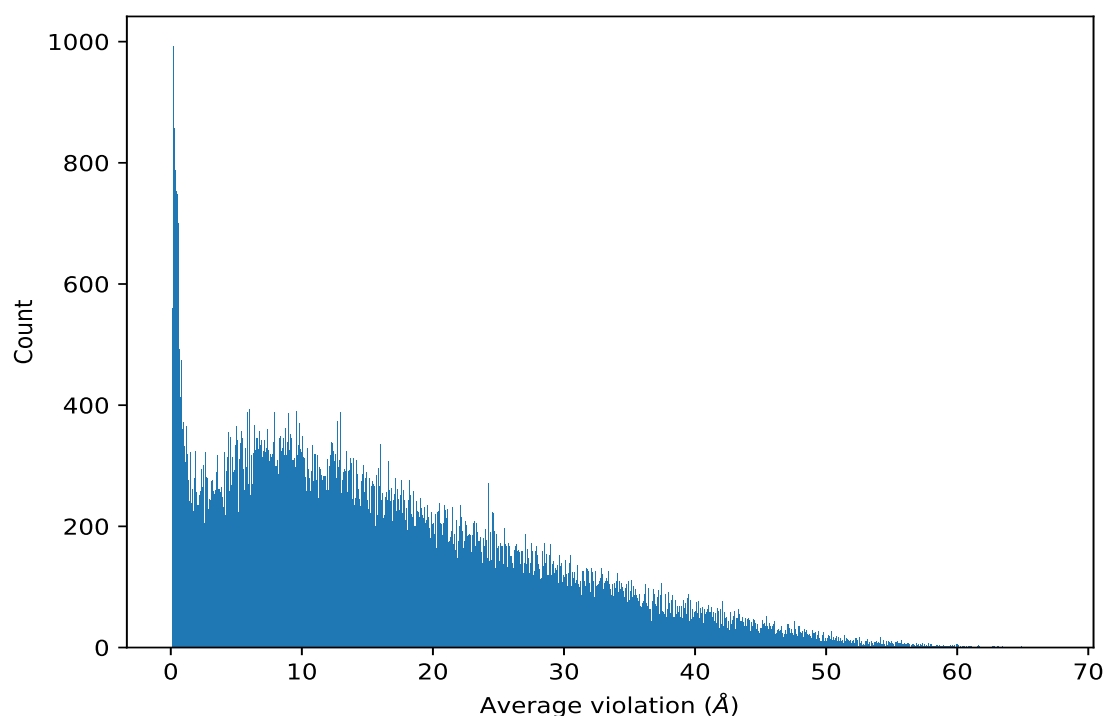
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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.

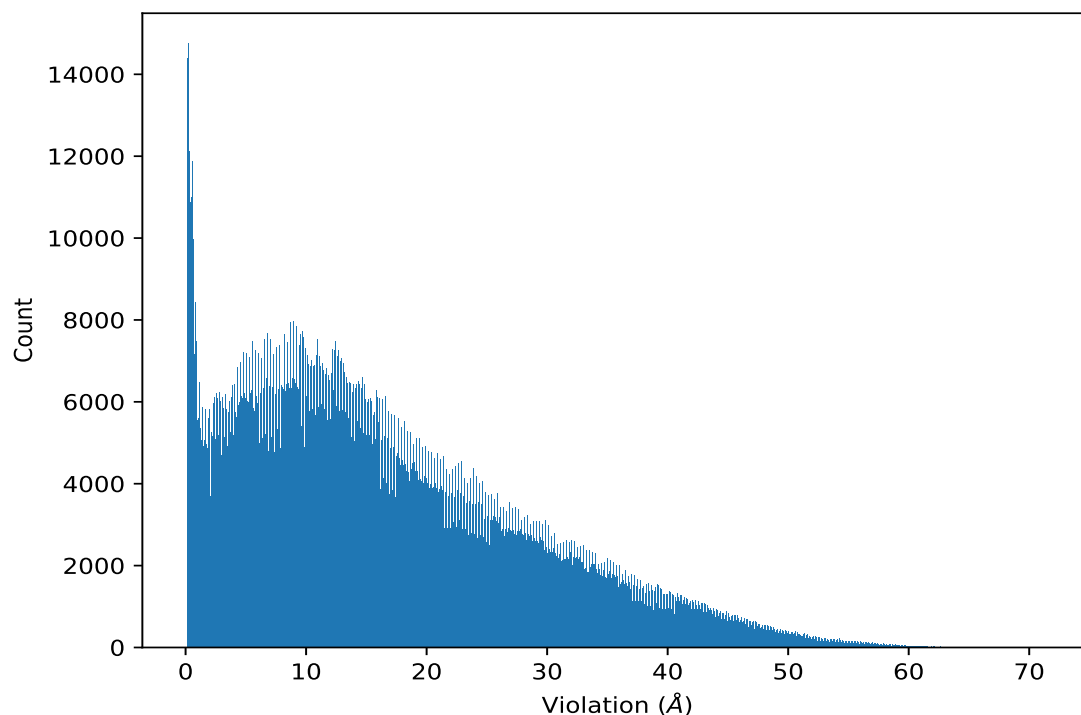
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,23946)	1:55:A:LEU:HG	1:125:A:LYS:HE2	20	67.0	3.18	66.88
(4,23894)	1:55:A:LEU:HG	1:125:A:LYS:HE3	20	66.94	3.16	67.51
(4,23362)	1:125:A:LYS:HD3	1:54:A:PRO:HB3	20	66.66	2.77	67.18
(4,23377)	1:125:A:LYS:HD2	1:54:A:PRO:HB3	20	66.28	2.78	66.84
(4,36247)	1:122:A:GLU:HB3	1:54:A:PRO:HB2	20	66.23	2.97	67.38
(4,23897)	1:55:A:LEU:HB3	1:125:A:LYS:HE2	20	65.95	2.11	66.07
(4,22110)	1:122:A:GLU:HB3	1:54:A:PRO:HB3	20	65.94	2.98	66.68
(4,23931)	1:55:A:LEU:HB3	1:125:A:LYS:HE3	20	65.88	2.1	66.18
(4,37055)	1:123:A:ASP:HB3	1:54:A:PRO:HA	20	65.46	2.65	65.88
(4,55821)	1:54:A:PRO:HG3	1:122:A:GLU:HA	20	65.06	2.69	65.72

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)
(4,23894)	1:55:A:LEU:HG	1:125:A:LYS:HE3	6	71.71
(4,23946)	1:55:A:LEU:HG	1:125:A:LYS:HE2	6	71.62
(4,23946)	1:55:A:LEU:HG	1:125:A:LYS:HE2	9	71.08
(4,23894)	1:55:A:LEU:HG	1:125:A:LYS:HE3	11	70.87
(4,23946)	1:55:A:LEU:HG	1:125:A:LYS:HE2	11	70.84
(4,23894)	1:55:A:LEU:HG	1:125:A:LYS:HE3	9	70.55
(4,23894)	1:55:A:LEU:HG	1:125:A:LYS:HE3	10	70.51
(4,23946)	1:55:A:LEU:HG	1:125:A:LYS:HE2	1	70.39
(4,23946)	1:55:A:LEU:HG	1:125:A:LYS:HE2	10	70.38
(4,23362)	1:125:A:LYS:HD3	1:54:A:PRO:HB3	1	70.16

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found