



wwPDB NMR Structure Validation Summary Report ⓘ

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BMRB ID : 17701
Title : B. subtilis L,D-transpeptidase
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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 : 4-5-2 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

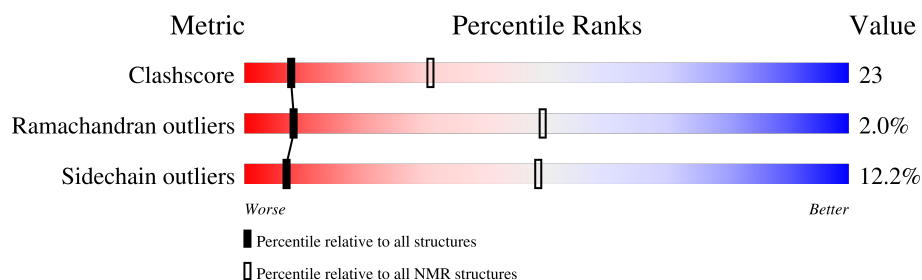
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 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	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	175	47% 38% 6% 6% .

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:4-A:107, A:113-A:167 (159)	0.27	7

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 4 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2597 atoms, of which 1322 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called L, D-TRANSPEPTIDASE YKUD.

Mol	Chain	Residues	Atoms						Trace
1	A	169	Total	C	H	N	O	S	0
			2597	810	1322	230	232	3	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP O34816
A	2	ARG	-	expression tag	UNP O34816
A	3	LYS	-	expression tag	UNP O34816
A	4	LEU	-	expression tag	UNP O34816
A	168	GLY	-	expression tag	UNP O34816
A	169	SER	-	expression tag	UNP O34816
A	170	HIS	-	expression tag	UNP O34816
A	171	HIS	-	expression tag	UNP O34816
A	172	HIS	-	expression tag	UNP O34816
A	173	HIS	-	expression tag	UNP O34816
A	174	HIS	-	expression tag	UNP O34816
A	175	HIS	-	expression tag	UNP O34816

5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *MINIMAL ENERGY*.

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

Software name	Classification	Version
CNS	refinement	1.2
NMRDraw	structure solution	
NMRPipe	structure solution	
CcpNmr Analysis	structure solution	2.1

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	2093
Number of shifts mapped to atoms	2084
Number of unparsed shifts	0
Number of shifts with mapping errors	9
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	0.68±0.01	0±0/1237 (0.0± 0.0%)	1.03±0.01	2±1/1688 (0.1± 0.0%)
All	All	0.68	0/24718 (0.0%)	1.03	32/33730 (0.1%)

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	0.3±0.6
All	All	0	7

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	123	TYR	CA-C-N	-8.29	116.46	122.18	4	16
1	A	123	TYR	C-N-CA	-8.29	116.46	122.18	4	16

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	103	ARG	Sidechain	6
1	A	105	ARG	Peptide	1

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	1212	1258	1257	55±8
All	All	24240	25160	24454	1106

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 23.

5 of 194 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:ALA:O	1:A:143:ILE:HA	0.84	1.73	3	19
1:A:123:TYR:O	1:A:143:ILE:HG12	0.83	1.73	20	1
1:A:103:ARG:NH2	1:A:158:PRO:HA	0.83	1.89	9	10
1:A:88:LYS:HG3	1:A:139:SER:O	0.79	1.77	18	2
1:A:89:ILE:HG23	1:A:90:LEU:HD22	0.77	1.57	15	19

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	159/175 (91%)	143±5 (90±3%)	12±1 (8±1%)	3±0 (2±0%)	8	49
All	All	3153/3500 (90%)	2851 (90%)	239 (8%)	63 (2%)	8	49

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	88	LYS	20
1	A	113	ALA	20
1	A	143	ILE	17

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Mol	Chain	Res	Type	Models (Total)
1	A	124	GLY	4
1	A	13	ASP	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	133/144 (92%)	111±25 (83±19%)	15±4 (12±3%)	8	50
All	All	2524/2880 (88%)	2217 (88%)	307 (12%)	7	48

5 of 38 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	6	THR	19
1	A	14	THR	19
1	A	40	LEU	19
1	A	74	LEU	19
1	A	89	ILE	19

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 92% for the well-defined parts and 92% 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	2093
Number of shifts mapped to atoms	2084
Number of unparsed shifts	0
Number of shifts with mapping errors	9
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 9) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	170	HIS	C	173.981	.	1
1	A	170	HIS	CA	55.85	.	1
1	A	171	HIS	H	8.084	0.095	1
1	A	171	HIS	C	174.055	.	1
1	A	171	HIS	CA	57.293	.	1
1	A	171	HIS	CB	30.293	.	1
1	A	171	HIS	N	125.398	0.045	1
1	A	172	HIS	H	7.958	0.006	1
1	A	172	HIS	N	125.204	0.004	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
$^{13}\text{C}_\alpha$	171	-0.09 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	152	-0.06 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	169	0.19 ± 0.10	None needed (< 0.5 ppm)
^{15}N	159	0.21 ± 0.27	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. 1999 atoms were assigned a chemical shift out of a possible 2165. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	785/787 (100%)	319/320 (100%)	317/318 (100%)	149/149 (100%)
Sidechain	1109/1251 (89%)	760/824 (92%)	330/379 (87%)	19/48 (40%)
Aromatic	105/127 (83%)	50/60 (83%)	46/58 (79%)	9/9 (100%)
Overall	1999/2165 (92%)	1129/1204 (94%)	693/755 (92%)	177/206 (86%)

7.1.4 Statistically unusual chemical shifts [i](#)

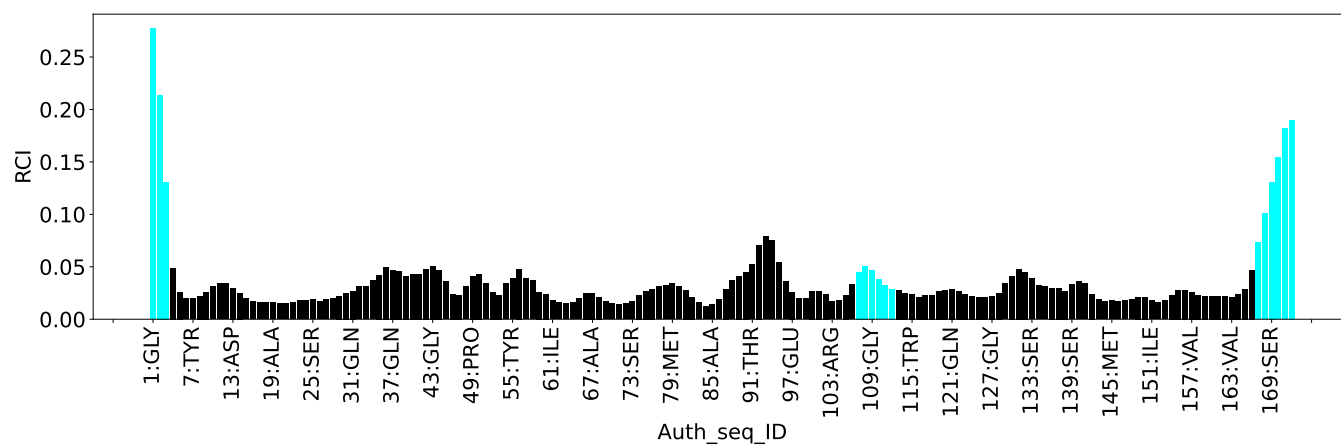
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	142	CYS	H	12.39	5.02 – 11.74	6.0

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	4901
Intra-residue ($ i-j =0$)	3458
Sequential ($ i-j =1$)	1205
Medium range ($ i-j >1$ and $ i-j <5$)	29
Long range ($ i-j \geq 5$)	209
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	28.0
Number of long range restraints per residue ¹	1.2

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)	152.8	0.2
0.2-0.5 (Medium)	533.8	0.5
>0.5 (Large)	3037.3	29.31

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 ⓘ

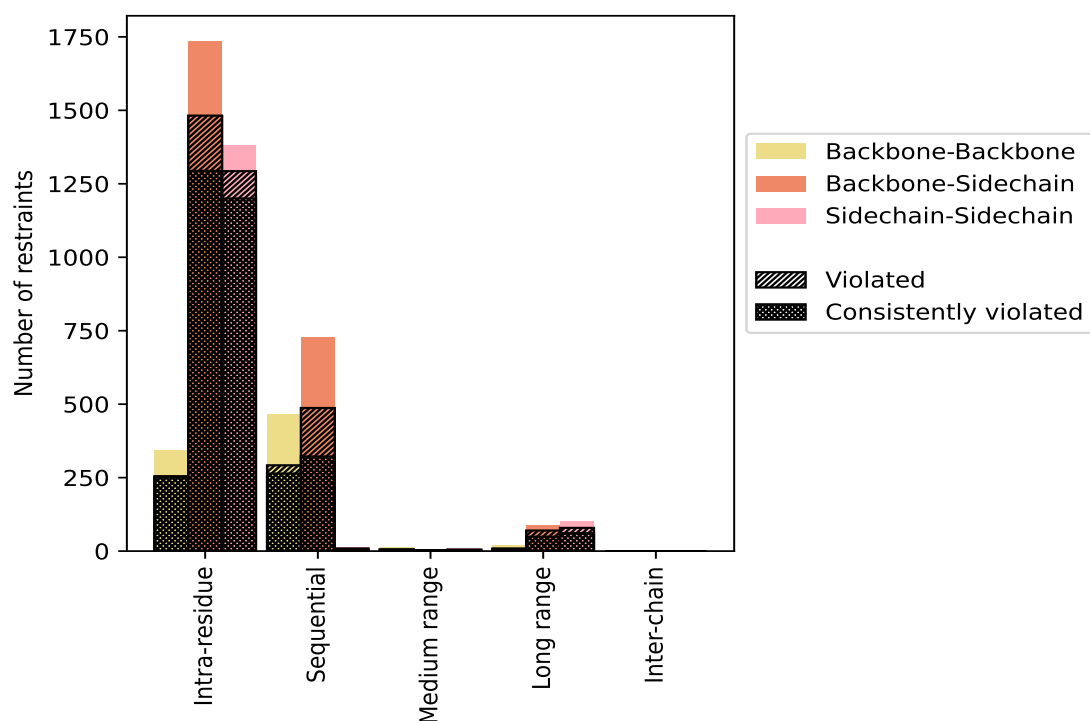
9.1 Summary of distance violations ⓘ

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)	3458	70.6	3030	87.6	61.8	2744	79.4	56.0
Backbone-Backbone	344	7.0	255	74.1	5.2	250	72.7	5.1
Backbone-Sidechain	1735	35.4	1482	85.4	30.2	1294	74.6	26.4
Sidechain-Sidechain	1379	28.1	1293	93.8	26.4	1200	87.0	24.5
Sequential (i-j =1)	1205	24.6	788	65.4	16.1	589	48.9	12.0
Backbone-Backbone	466	9.5	292	62.7	6.0	264	56.7	5.4
Backbone-Sidechain	728	14.9	487	66.9	9.9	322	44.2	6.6
Sidechain-Sidechain	11	0.2	9	81.8	0.2	3	27.3	0.1
Medium range (i-j >1 & i-j <5)	29	0.6	14	48.3	0.3	12	41.4	0.2
Backbone-Backbone	13	0.3	6	46.2	0.1	5	38.5	0.1
Backbone-Sidechain	7	0.1	3	42.9	0.1	3	42.9	0.1
Sidechain-Sidechain	9	0.2	5	55.6	0.1	4	44.4	0.1
Long range (i-j ≥5)	209	4.3	158	75.6	3.2	117	56.0	2.4
Backbone-Backbone	21	0.4	9	42.9	0.2	7	33.3	0.1
Backbone-Sidechain	88	1.8	70	79.5	1.4	49	55.7	1.0
Sidechain-Sidechain	100	2.0	79	79.0	1.6	61	61.0	1.2
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	4901	100.0	3990	81.4	81.4	3462	70.6	70.6
Backbone-Backbone	844	17.2	562	66.6	11.5	526	62.3	10.7
Backbone-Sidechain	2558	52.2	2042	79.8	41.7	1668	65.2	34.0
Sidechain-Sidechain	1499	30.6	1386	92.5	28.3	1268	84.6	25.9

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 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	2890	680	14	138	0	3722	1.2	28.4	0.84	1.15
2	2905	685	14	136	0	3740	1.2	28.01	0.84	1.14
3	2905	677	13	139	0	3734	1.2	28.1	0.84	1.14
4	2898	682	13	138	0	3731	1.2	28.34	0.84	1.15
5	2898	679	13	138	0	3728	1.2	28.24	0.84	1.14
6	2900	676	13	138	0	3727	1.2	28.03	0.84	1.14
7	2903	684	14	137	0	3738	1.2	28.72	0.84	1.14
8	2891	681	13	136	0	3721	1.2	28.13	0.84	1.14
9	2906	682	13	131	0	3732	1.2	28.98	0.85	1.15
10	2901	677	14	137	0	3729	1.2	28.03	0.84	1.14

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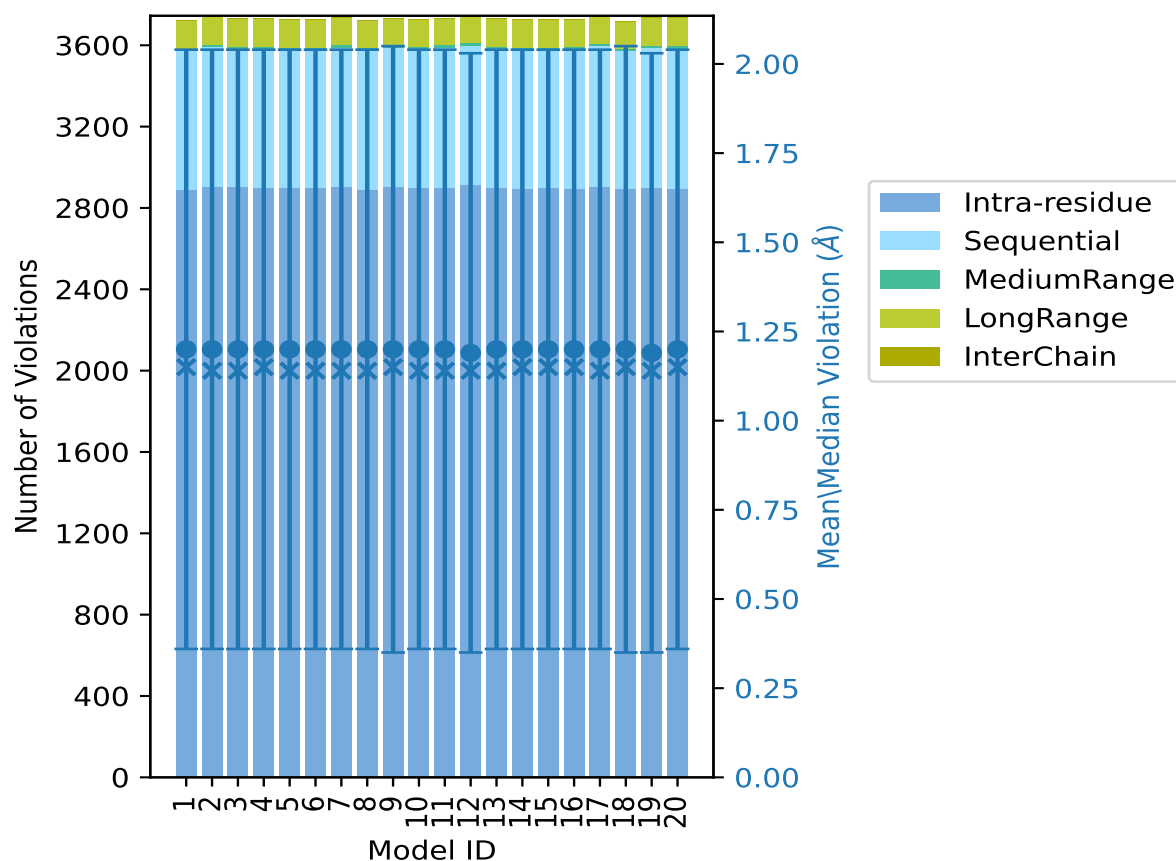
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	2898	688	14	132	0	3732	1.2	27.58	0.84	1.14
12	2914	684	14	133	0	3745	1.19	28.84	0.84	1.14
13	2901	679	13	138	0	3731	1.2	27.66	0.84	1.14
14	2896	681	14	138	0	3729	1.2	28.05	0.84	1.15
15	2898	679	13	135	0	3725	1.2	28.57	0.84	1.15
16	2894	683	14	136	0	3727	1.2	28.13	0.84	1.15
17	2906	689	13	137	0	3745	1.2	27.78	0.84	1.14
18	2897	674	14	134	0	3719	1.2	29.31	0.85	1.15
19	2899	686	14	137	0	3736	1.19	28.1	0.84	1.14
20	2893	689	14	140	0	3736	1.2	27.97	0.84	1.15

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

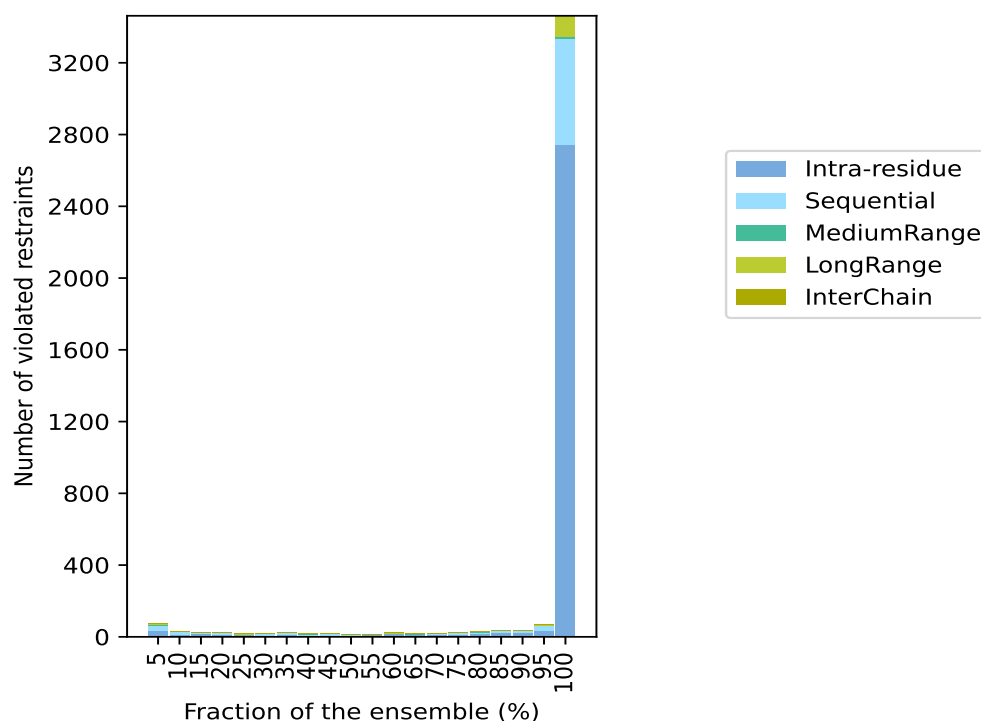
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 911(IR:428, SQ:417, MR:15, LR:51, IC:0) restraints are not 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	%
32	33	0	8	0	73	1	5.0
13	17	0	2	0	32	2	10.0
17	8	0	1	0	26	3	15.0
10	13	0	3	0	26	4	20.0
10	4	0	2	0	16	5	25.0
8	8	0	2	0	18	6	30.0
11	11	0	0	0	22	7	35.0
8	7	0	2	0	17	8	40.0
8	9	0	2	0	19	9	45.0
7	7	0	1	0	15	10	50.0
8	5	0	0	0	13	11	55.0
17	3	0	2	0	22	12	60.0
12	3	1	2	0	18	13	65.0
13	5	0	2	0	20	14	70.0
13	9	0	1	0	23	15	75.0
19	8	0	2	0	29	16	80.0
22	11	0	0	0	33	17	85.0
22	12	1	1	0	36	18	90.0
36	26	0	8	0	70	19	95.0
2744	589	12	117	0	3462	20	100.0

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

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

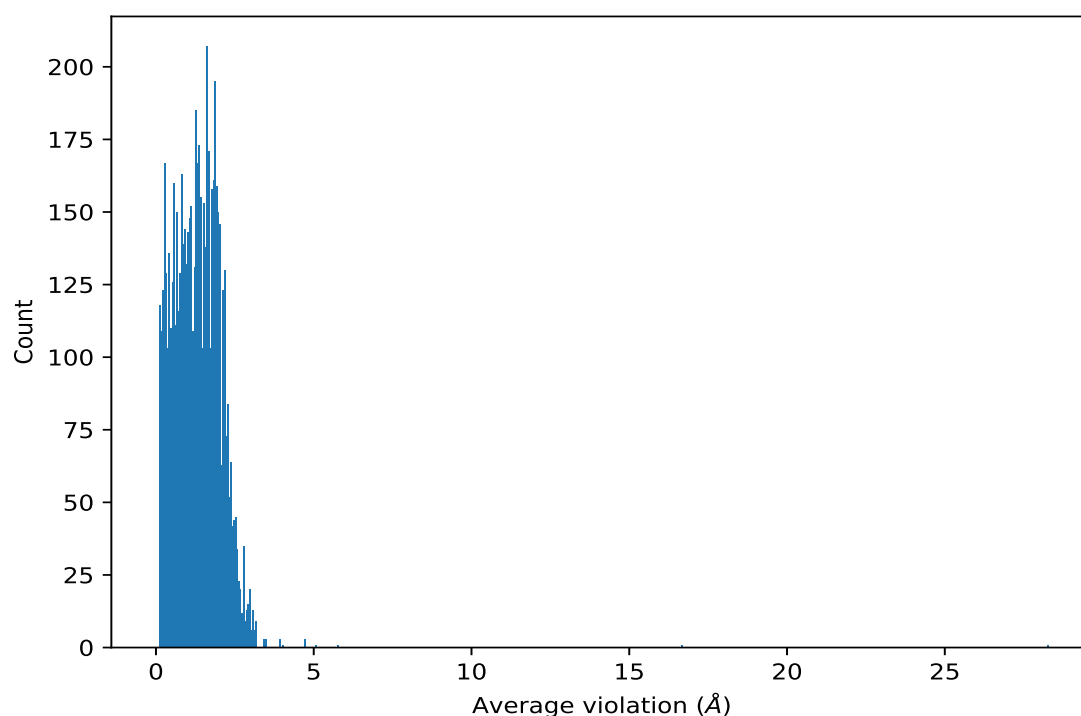
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(2,2053)	1:34:A:PRO:HG2	1:94:A:PRO:HB2	20	28.25	0.43	28.12
(2,1296)	1:40:A:LEU:HB2	1:90:A:LEU:HA	20	16.66	0.3	16.61
(2,2029)	1:110:A:PRO:HA	1:107:A:PRO:HA	20	5.75	0.1	5.76
(2,2720)	1:97:A:GLU:HA	1:60:A:HIS:HA	20	5.06	0.16	5.06
(2,1912)	1:74:A:LEU:HD21	1:75:A:ASN:H	20	4.72	0.03	4.73
(2,1912)	1:74:A:LEU:HD22	1:75:A:ASN:H	20	4.72	0.03	4.73
(2,1912)	1:74:A:LEU:HD23	1:75:A:ASN:H	20	4.72	0.03	4.73
(4,1481)	1:114:A:TYR:HA	1:115:A:TRP:HE1	20	4.04	0.07	4.04
(2,53)	1:103:A:ARG:HG2	1:116:A:LEU:HD21	20	3.93	0.51	4.05
(2,53)	1:103:A:ARG:HG2	1:116:A:LEU:HD22	20	3.93	0.51	4.05
(2,53)	1:103:A:ARG:HG2	1:116:A:LEU:HD23	20	3.93	0.51	4.05
(2,1117)	1:165:A:ILE:HD11	1:165:A:ILE:H	20	3.49	0.02	3.49
(2,1117)	1:165:A:ILE:HD12	1:165:A:ILE:H	20	3.49	0.02	3.49
(2,1117)	1:165:A:ILE:HD13	1:165:A:ILE:H	20	3.49	0.02	3.49
(2,1245)	1:134:A:ILE:HG13	1:134:A:ILE:HG21	20	3.44	0.01	3.44
(2,1245)	1:134:A:ILE:HG13	1:134:A:ILE:HG22	20	3.44	0.01	3.44

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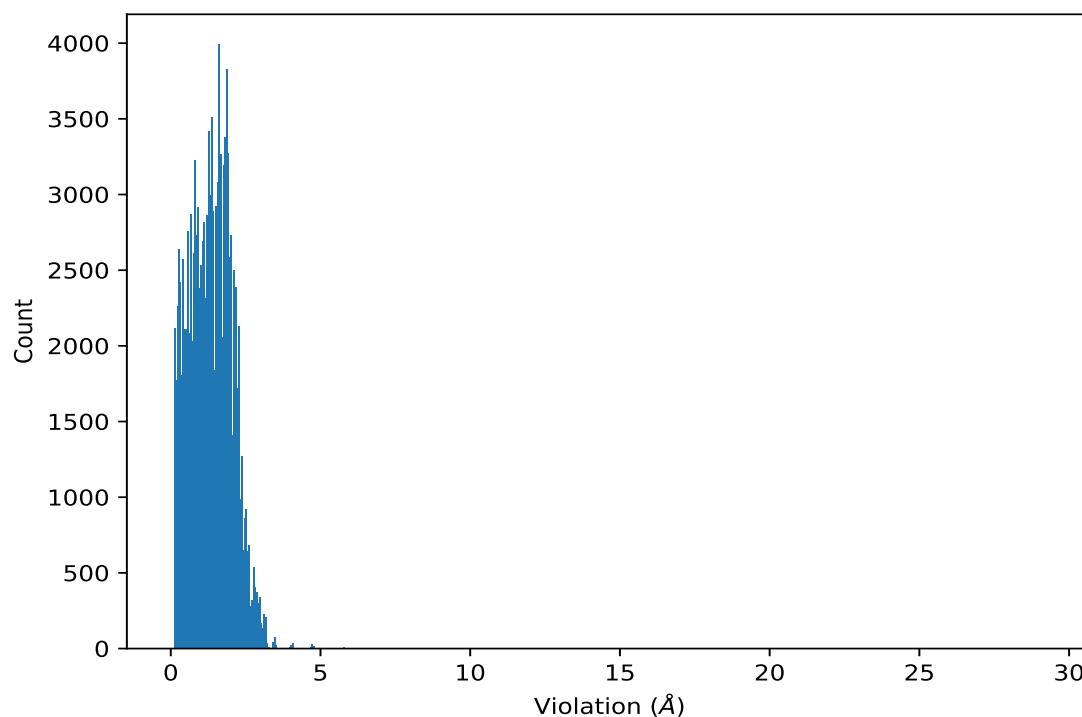
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1245)	1:134:A:ILE:HG13	1:134:A:ILE:HG23	20	3.44	0.01	3.44
(2,539)	1:134:A:ILE:HD11	1:134:A:ILE:HG13	20	3.18	0.0	3.18

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)
(2,2053)	1:34:A:PRO:HG2	1:94:A:PRO:HB2	18	29.31
(2,2053)	1:34:A:PRO:HG2	1:94:A:PRO:HB2	9	28.98
(2,2053)	1:34:A:PRO:HG2	1:94:A:PRO:HB2	12	28.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2053)	1:34:A:PRO:HG2	1:94:A:PRO:HB2	7	28.72
(2,2053)	1:34:A:PRO:HG2	1:94:A:PRO:HB2	15	28.57
(2,2053)	1:34:A:PRO:HG2	1:94:A:PRO:HB2	1	28.4
(2,2053)	1:34:A:PRO:HG2	1:94:A:PRO:HB2	4	28.34
(2,2053)	1:34:A:PRO:HG2	1:94:A:PRO:HB2	5	28.24
(2,2053)	1:34:A:PRO:HG2	1:94:A:PRO:HB2	8	28.13
(2,2053)	1:34:A:PRO:HG2	1:94:A:PRO:HB2	16	28.13

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found