



wwPDB NMR Structure Validation Summary Report ⓘ

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

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<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

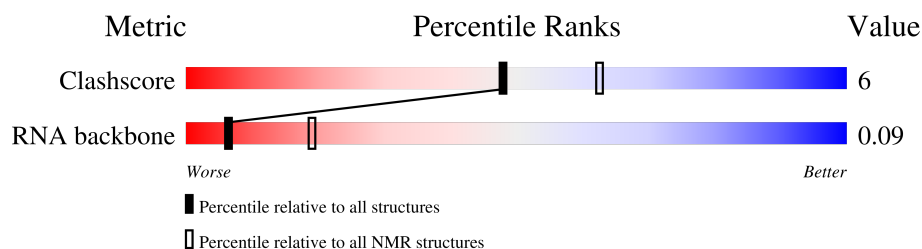
1 Overall quality at a glance

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
RNA backbone	8273	777

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	14	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 460 atoms, of which 155 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called RNA hairpin with GAAG tetraloop.


Mol	Chain	Residues	Atoms						Trace
1	A	14	Total	C	H	N	O	P	0
			460	135	155	59	97	14	

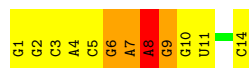
4 Residue-property plots

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: RNA hairpin with GAAG tetraloop


Chain A: 



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

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: RNA hairpin with GAAG tetraloop

Chain A: 



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure calculation	
ARIA	structure calculation	

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	327
Number of shifts mapped to atoms	327
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

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	0.41±0.01	1±0/341 (0.3± 0.0%)	0.76±0.03	1±0/529 (0.2± 0.1%)
All	All	0.41	20/6820 (0.3%)	0.76	17/10580 (0.2%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.1±0.2
All	All	0	21

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	1	G	OP3-P	5.59	1.59	1.48	10	20

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	8	A	C2'-C3'-O3'	5.66	117.98	109.50	10	17

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	7	A	Sidechain	20
1	A	5	C	Sidechain	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	305	155	154	3±1
All	All	6100	3100	3080	54

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 6.

5 of 8 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:A:C2	1:A:9:G:C8	0.68	2.82	10	20
1:A:5:C:H2'	1:A:6:G:C8	0.53	2.38	17	16
1:A:6:G:N3	1:A:8:A:C8	0.46	2.84	10	1
1:A:7:A:C6	1:A:8:A:C5	0.46	3.04	10	4
1:A:8:A:N3	1:A:9:G:C8	0.42	2.87	10	8

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

6.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

6.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	13/14 (93%)	10±0 (77±0%)	1±0 (8±2%)	0.17±0.00
All	All	260/280 (93%)	200 (77%)	21 (8%)	0.17

The overall RNA backbone suiteness is 0.09.

5 of 10 unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	2	G	20
1	A	3	C	20
1	A	4	A	20
1	A	6	G	20
1	A	7	A	20

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	8	A	20
1	A	7	A	1

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 [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: *starch_output*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	327
Number of shifts mapped to atoms	327
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

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. 248 atoms were assigned a chemical shift out of a possible 289. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Sugar	153/154 (99%)	83/84 (99%)	70/70 (100%)	0/0 (—%)
Base	95/135 (70%)	35/74 (47%)	21/22 (95%)	39/39 (100%)
Overall	248/289 (86%)	118/158 (75%)	91/92 (99%)	39/39 (100%)

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 con-

taining paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, <i>ppm</i>	Expected range, <i>ppm</i>	Z-score
1	A	8	A	N3	126.50	196.84 – 232.12	-24.9

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

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins

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	927
Intra-residue ($ i-j =0$)	559
Sequential ($ i-j =1$)	291
Medium range ($ i-j >1$ and $ i-j <5$)	18
Long range ($ i-j \geq 5$)	31
Inter-chain	0
Hydrogen bond restraints	28
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	66.2
Number of long range restraints per residue ¹	4.2

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)	7.8	0.2
0.2-0.5 (Medium)	17.4	0.5
>0.5 (Large)	853.2	4.66

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 ⓘ

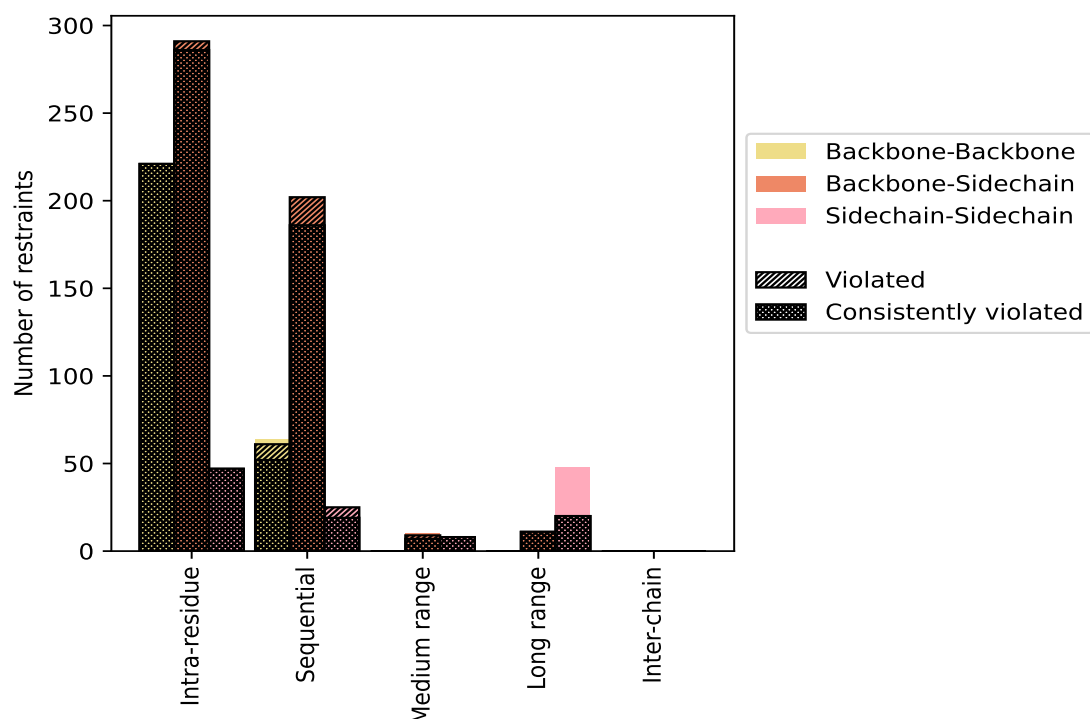
9.1 Summary of distance violations ⓘ

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)	559	60.3	559	100.0	60.3	554	99.1	59.8
Backbone-Backbone	221	23.8	221	100.0	23.8	221	100.0	23.8
Backbone-Sidechain	291	31.4	291	100.0	31.4	286	98.3	30.9
Sidechain-Sidechain	47	5.1	47	100.0	5.1	47	100.0	5.1
Sequential (i-j =1)	291	31.4	288	99.0	31.1	257	88.3	27.7
Backbone-Backbone	64	6.9	61	95.3	6.6	52	81.2	5.6
Backbone-Sidechain	202	21.8	202	100.0	21.8	186	92.1	20.1
Sidechain-Sidechain	25	2.7	25	100.0	2.7	19	76.0	2.0
Medium range (i-j >1 & i-j <5)	18	1.9	17	94.4	1.8	15	83.3	1.6
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	10	1.1	9	90.0	1.0	7	70.0	0.8
Sidechain-Sidechain	8	0.9	8	100.0	0.9	8	100.0	0.9
Long range (i-j ≥5)	31	3.3	31	100.0	3.3	31	100.0	3.3
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	11	1.2	11	100.0	1.2	11	100.0	1.2
Sidechain-Sidechain	20	2.2	20	100.0	2.2	20	100.0	2.2
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	28	3.0	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	927	100.0	895	96.5	96.5	857	92.4	92.4
Backbone-Backbone	285	30.7	282	98.9	30.4	273	95.8	29.4
Backbone-Sidechain	514	55.4	513	99.8	55.3	490	95.3	52.9
Sidechain-Sidechain	128	13.8	100	78.1	10.8	94	73.4	10.1

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	558	276	17	31	0	882	2.61	4.65	1.07	2.67
2	555	267	16	31	0	869	2.65	4.65	1.05	2.69
3	557	275	16	31	0	879	2.6	4.65	1.07	2.66
4	559	274	16	31	0	880	2.6	4.66	1.06	2.68
5	558	272	16	31	0	877	2.61	4.66	1.05	2.68
6	556	277	16	31	0	880	2.62	4.66	1.07	2.71
7	557	272	16	31	0	876	2.63	4.65	1.05	2.68
8	558	273	16	31	0	878	2.62	4.66	1.05	2.68
9	557	274	16	31	0	878	2.63	4.66	1.05	2.69
10	557	275	15	31	0	878	2.61	4.65	1.05	2.66

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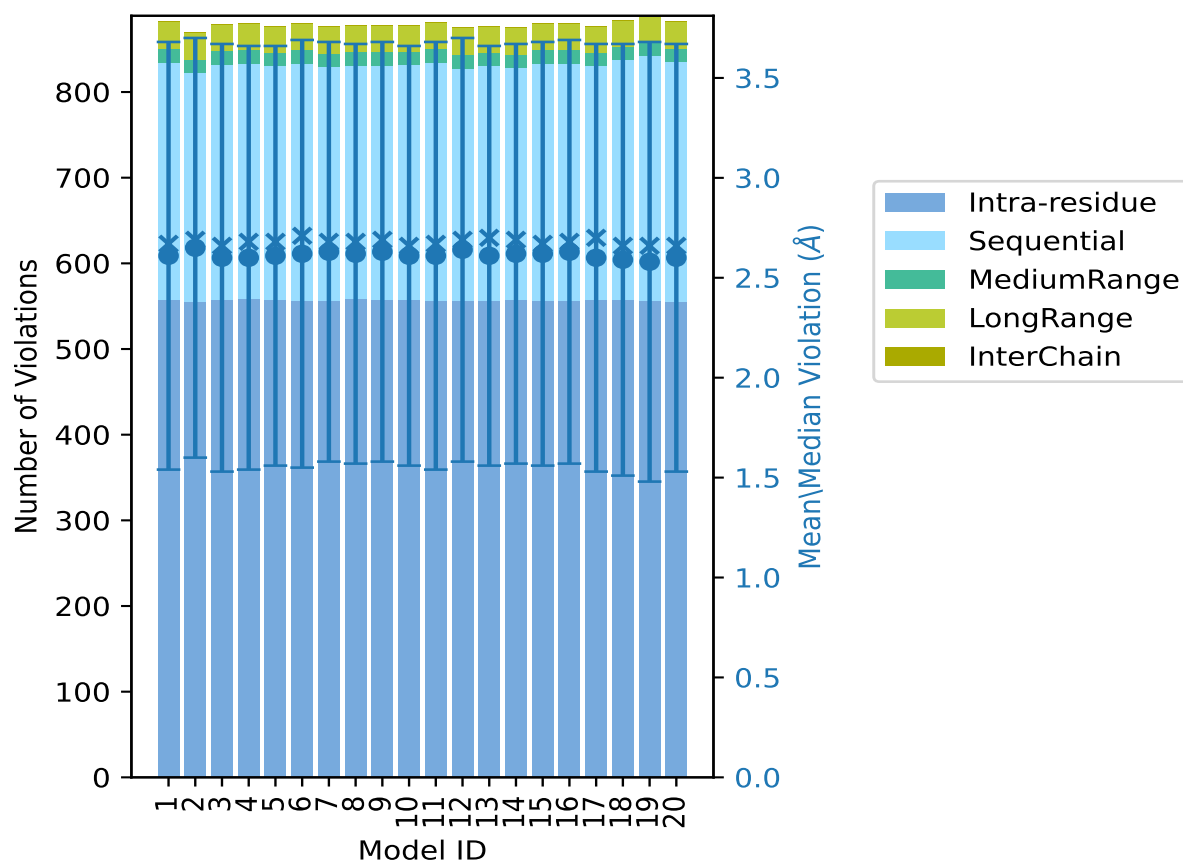
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	557	277	16	31	0	881	2.61	4.66	1.07	2.67
12	557	270	17	31	0	875	2.64	4.65	1.06	2.69
13	556	274	16	31	0	877	2.61	4.66	1.05	2.7
14	558	270	16	31	0	875	2.62	4.66	1.05	2.69
15	556	277	16	31	0	880	2.62	4.66	1.06	2.67
16	556	277	16	31	0	880	2.63	4.65	1.06	2.68
17	557	273	16	31	0	877	2.6	4.65	1.07	2.7
18	557	281	15	31	0	884	2.59	4.66	1.08	2.66
19	557	285	16	31	0	889	2.58	4.65	1.1	2.66
20	556	279	16	31	0	882	2.6	4.66	1.07	2.66

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 ⓘ

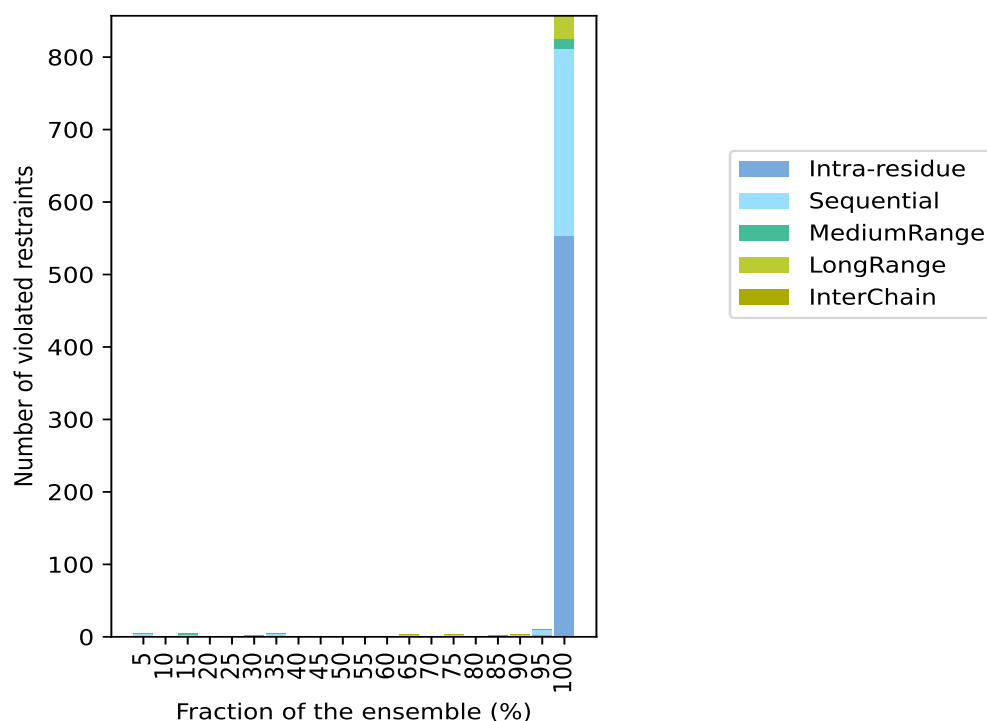
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 4(IR:0, SQ:3, MR:1, LR:0, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	5	0	0	0	5	1	5.0
0	0	0	0	0	0	2	10.0
1	2	1	0	0	4	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	2	0	0	0	2	6	30.0
0	4	0	0	0	4	7	35.0
1	0	0	0	0	1	8	40.0
0	0	0	0	0	0	9	45.0
1	0	0	0	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	3	0	0	0	3	13	65.0
0	0	0	0	0	0	14	70.0
0	3	0	0	0	3	15	75.0
0	0	0	0	0	0	16	80.0
0	1	1	0	0	2	17	85.0
0	3	0	0	0	3	18	90.0
2	8	0	0	0	10	19	95.0
554	257	15	31	0	857	20	100.0

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

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

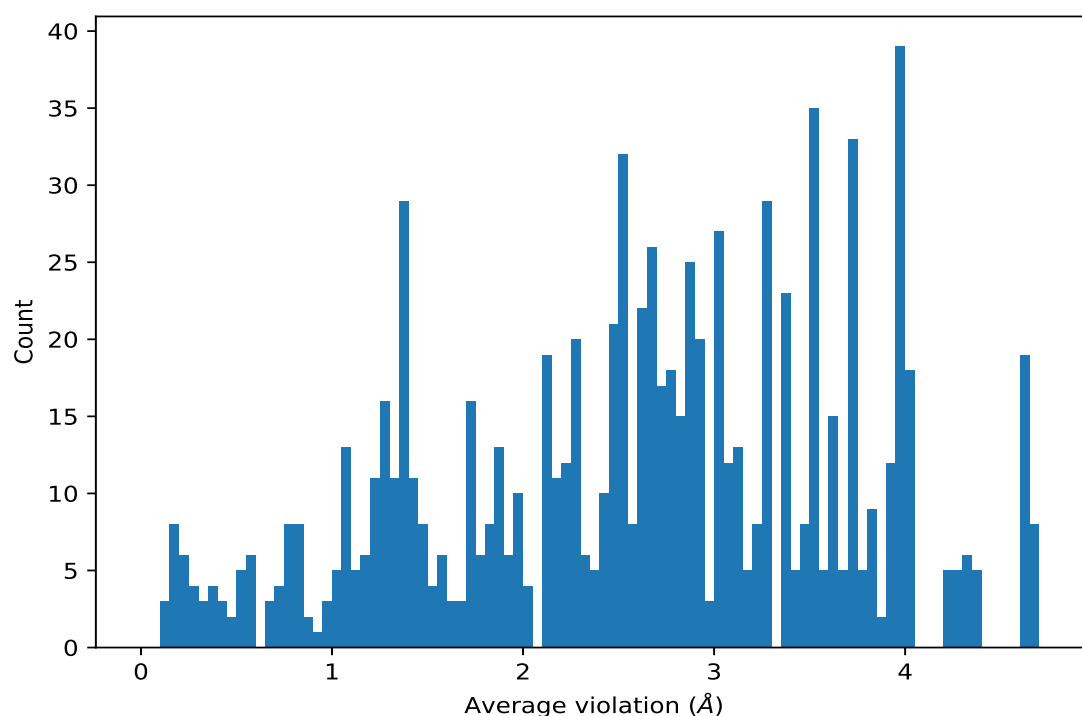
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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.

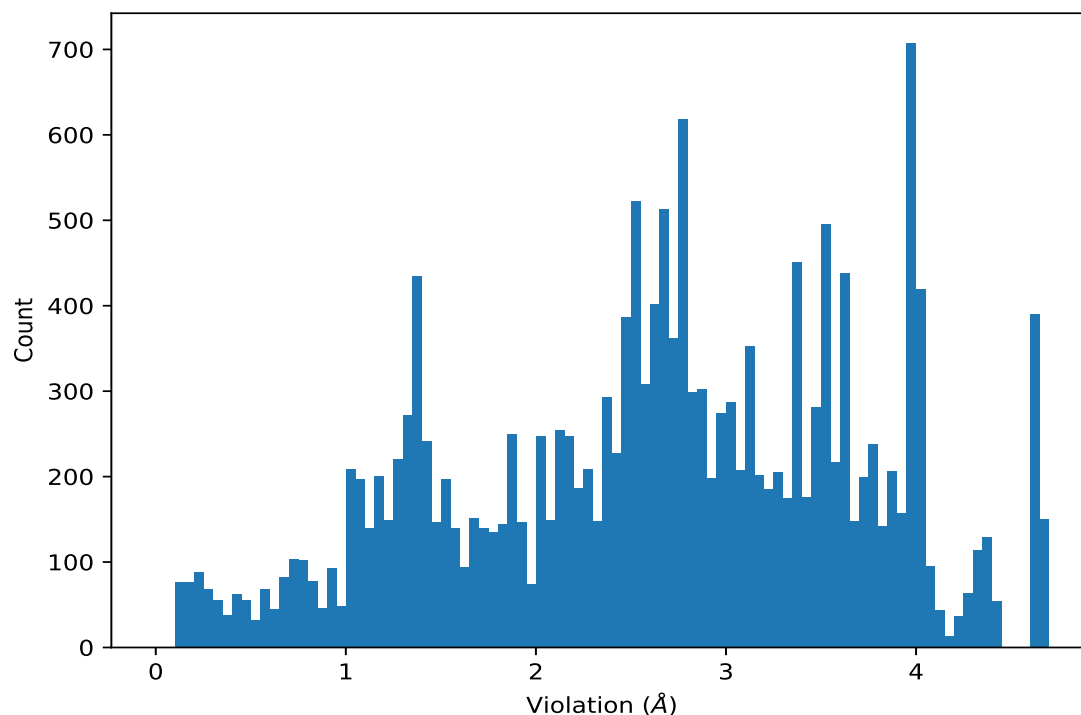
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,47)	1:5:A:C:H42	1:5:A:C:H41	20	4.66	0.0	4.66
(5,44)	1:5:A:C:H42	1:5:A:C:H41	20	4.66	0.0	4.66
(3,23)	1:3:A:C:H42	1:3:A:C:H41	20	4.65	0.0	4.65
(5,23)	1:3:A:C:H42	1:3:A:C:H41	20	4.65	0.0	4.65
(3,155)	1:13:A:C:H42	1:13:A:C:H41	20	4.65	0.0	4.65
(5,115)	1:13:A:C:H42	1:13:A:C:H41	20	4.65	0.0	4.65
(3,168)	1:14:A:C:H42	1:14:A:C:H41	20	4.65	0.0	4.65
(5,126)	1:14:A:C:H42	1:14:A:C:H41	20	4.65	0.0	4.65
(1,103)	1:7:A:A:H5''	1:7:A:A:H5'	20	4.63	0.0	4.63
(2,88)	1:7:A:A:H5''	1:7:A:A:H5'	20	4.63	0.0	4.63

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)
(5,44)	1:5:A:C:H42	1:5:A:C:H41	4	4.66
(5,44)	1:5:A:C:H42	1:5:A:C:H41	5	4.66
(5,44)	1:5:A:C:H42	1:5:A:C:H41	6	4.66
(5,44)	1:5:A:C:H42	1:5:A:C:H41	8	4.66
(5,44)	1:5:A:C:H42	1:5:A:C:H41	9	4.66
(5,44)	1:5:A:C:H42	1:5:A:C:H41	11	4.66
(5,44)	1:5:A:C:H42	1:5:A:C:H41	13	4.66
(5,44)	1:5:A:C:H42	1:5:A:C:H41	14	4.66
(5,44)	1:5:A:C:H42	1:5:A:C:H41	15	4.66
(5,44)	1:5:A:C:H42	1:5:A:C:H41	18	4.66

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found