



# wwPDB NMR Structure Validation Summary Report ⓘ

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BMRB ID : 35023  
Title : Beyond single-state RNA structural biology: MD/NMR description of temperature-sensitive dynamic RNA ensembles - GCAA MD conformational ensemble  
Authors : Leopold, D.; Oxenfarth, A.; Thomasen, F.E.; Kuemmerer, F.; Schnieders, R.; Pinter, G.; Wacker, A.; Jonker, H.R.A.; Fuertig, B.; Richter, C.; Lindorff-Larsen, K.; Schwalbe, H.  
Deposited on : 2025-10-11

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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

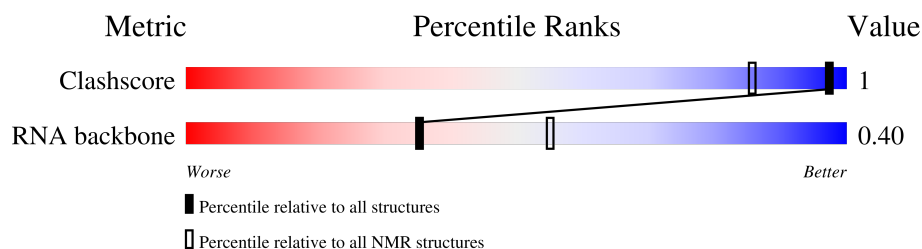
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*


The overall completeness of chemical shifts assignment is 75%.

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  $\geq 3$ , 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	 79% 21%

## 2 Ensemble composition and analysis ⓘ

This entry contains 100 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 453 atoms, of which 155 are hydrogens and 0 are deuteriums.

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


Mol	Chain	Residues	Atoms						Trace
1	A	14	Total	C	H	N	O	P	0
			453	134	155	57	94	13	

## 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 GCAA tetraloop

Chain A:  79% 21%



### 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 GCAA tetraloop

Chain A:  50% 50%



## 5 Refinement protocol and experimental data overview

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

Of the 20100 calculated structures, 100 were deposited, based on the following criterion: *back calculated data agree with NOE, RDC, j-couplings, CCR*.

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

Software name	Classification	Version
GROMACS	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	236
Number of shifts mapped to atoms	235
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	75%

## 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	1.91±0.08	5±2/333 ( 1.4± 0.7%)	2.02±0.09	17±4/518 ( 3.4± 0.8%)
All	All	1.91	477/33300 ( 1.4%)	2.02	1749/51800 ( 3.4%)

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	8.0±2.0
All	All	0	800

5 of 156 unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	7	C	O3'-P	-9.45	1.47	1.61	89	11
1	A	7	C	P-O5'	-9.10	1.46	1.59	76	2
1	A	14	C	O4'-C1'	9.03	1.55	1.41	87	1
1	A	13	C	C4'-O4'	-9.01	1.32	1.45	80	6
1	A	14	C	C4'-O4'	-8.98	1.32	1.45	21	11

5 of 229 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	8	A	C4'-C3'-C2'	-11.74	90.86	102.60	99	13
1	A	14	C	C4'-C3'-C2'	-11.12	91.48	102.60	64	15
1	A	2	G	O4'-C1'-N9	11.02	125.02	108.50	22	10
1	A	12	G	O4'-C4'-C3'	10.84	114.84	104.00	85	17
1	A	10	G	C3'-C2'-C1'	10.79	112.09	101.30	48	8

There are no chirality outliers.

5 of 14 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	12	G	Sidechain	78
1	A	6	G	Sidechain	72
1	A	10	G	Sidechain	71
1	A	1	G	Sidechain	67
1	A	2	G	Sidechain	61

## 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	298	155	149	0±1
All	All	29800	15500	14682	27

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 1.

5 of 21 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:A:C8	1:A:10:G:C8	0.52	2.97	49	1
1:A:2:G:C2	1:A:14:C:C2	0.50	3.00	16	1
1:A:13:C:C2	1:A:14:C:C6	0.48	3.02	9	1
1:A:5:C:N4	1:A:6:G:C6	0.47	2.83	4	1
1:A:5:C:C4	1:A:6:G:C4	0.47	3.03	71	1

## 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%)	1±0 (8±0%)	1±1 (4±5%)	0.45±0.00
All	All	1302/1400 (93%)	100 (8%)	51 (4%)	0.45

The overall RNA backbone suiteness is 0.40.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	10	G	100

5 of 11 unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	7	C	14
1	A	8	A	14
1	A	9	A	8
1	A	10	G	3
1	A	5	C	2

## 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 ⓘ

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 75% for the well-defined parts and 75% 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	236
Number of shifts mapped to atoms	235
Number of unparsed shifts	0
Number of shifts with mapping errors	1
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. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	G	P	-0.14	0.01	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 75%, i.e. 206 atoms were assigned a chemical shift out of a possible 273. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Sugar	149/154 (97%)	81/84 (96%)	68/70 (97%)	0/0 (—%)
Base	57/119 (48%)	26/73 (36%)	22/23 (96%)	9/23 (39%)
Overall	206/273 (75%)	107/157 (68%)	90/93 (97%)	9/23 (39%)

#### 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, <i>ppm</i>	Expected range, <i>ppm</i>	Z-score
1	A	1	G	N1	133.70	135.47 – 158.37	-5.8

#### 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	616
Intra-residue ( $ i-j =0$ )	402
Sequential ( $ i-j =1$ )	164
Medium range ( $ i-j >1$ and $ i-j <5$ )	4
Long range ( $ i-j \geq 5$ )	18
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	44.0
Number of long range restraints per residue <sup>1</sup>	3.3

<sup>1</sup>Long 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)	2.4	0.2
0.2-0.5 (Medium)	7.0	0.5
>0.5 (Large)	579.1	8.19

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

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations

## 9 Distance violation analysis ⓘ

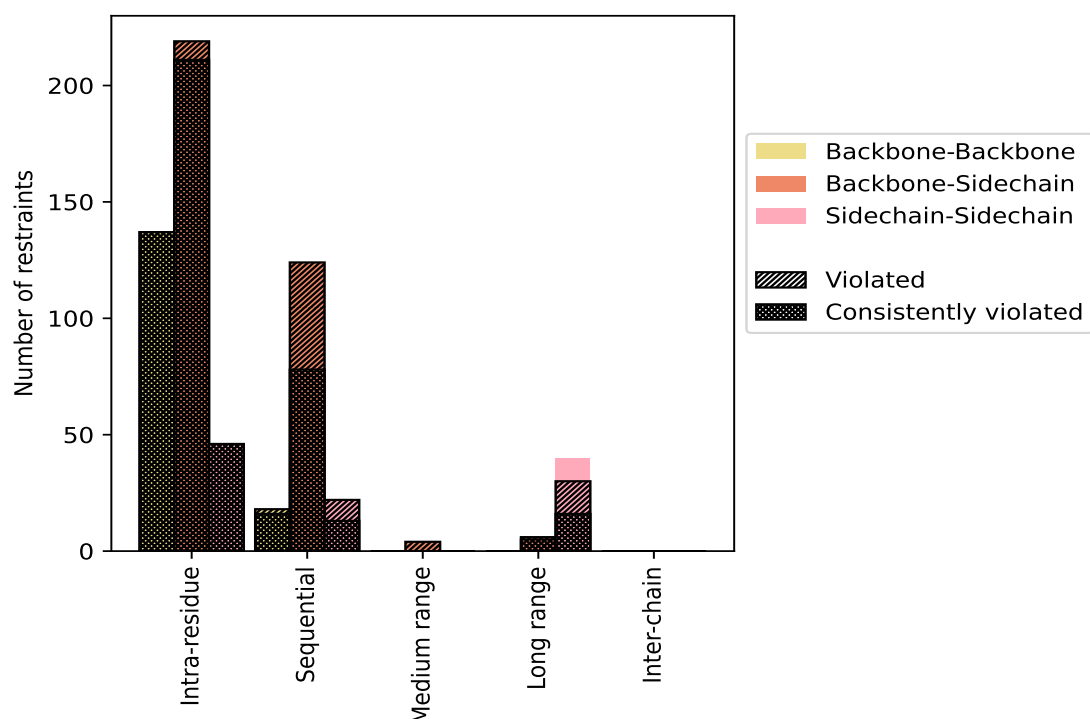
### 9.1 Summary of distance violations ⓘ

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	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<a href="#">Intra-residue ( i-j =0)</a>	<a href="#">402</a>	<a href="#">65.3</a>	<a href="#">402</a>	<a href="#">100.0</a>	<a href="#">65.3</a>	<a href="#">394</a>	<a href="#">98.0</a>	<a href="#">64.0</a>
Backbone-Backbone	137	22.2	137	100.0	22.2	137	100.0	22.2
Backbone-Sidechain	219	35.6	219	100.0	35.6	211	96.3	34.3
Sidechain-Sidechain	46	7.5	46	100.0	7.5	46	100.0	7.5
<a href="#">Sequential ( i-j =1)</a>	<a href="#">164</a>	<a href="#">26.6</a>	<a href="#">164</a>	<a href="#">100.0</a>	<a href="#">26.6</a>	<a href="#">107</a>	<a href="#">65.2</a>	<a href="#">17.4</a>
Backbone-Backbone	18	2.9	18	100.0	2.9	16	88.9	2.6
Backbone-Sidechain	124	20.1	124	100.0	20.1	78	62.9	12.7
Sidechain-Sidechain	22	3.6	22	100.0	3.6	13	59.1	2.1
<a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a>	<a href="#">4</a>	<a href="#">0.6</a>	<a href="#">4</a>	<a href="#">100.0</a>	<a href="#">0.6</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	4	0.6	4	100.0	0.6	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
<a href="#">Long range ( i-j ≥5)</a>	<a href="#">18</a>	<a href="#">2.9</a>	<a href="#">18</a>	<a href="#">100.0</a>	<a href="#">2.9</a>	<a href="#">17</a>	<a href="#">94.4</a>	<a href="#">2.8</a>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	6	1.0	6	100.0	1.0	5	83.3	0.8
Sidechain-Sidechain	12	1.9	12	100.0	1.9	12	100.0	1.9
<a href="#">Inter-chain</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
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
<a href="#">Hydrogen bond</a>	<a href="#">28</a>	<a href="#">4.5</a>	<a href="#">18</a>	<a href="#">64.3</a>	<a href="#">2.9</a>	<a href="#">4</a>	<a href="#">14.3</a>	<a href="#">0.6</a>
<a href="#">Disulfide bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Total</a>	<a href="#">616</a>	<a href="#">100.0</a>	<a href="#">606</a>	<a href="#">98.4</a>	<a href="#">98.4</a>	<a href="#">522</a>	<a href="#">84.7</a>	<a href="#">84.7</a>
Backbone-Backbone	155	25.2	155	100.0	25.2	153	98.7	24.8
Backbone-Sidechain	353	57.3	353	100.0	57.3	294	83.3	47.7
Sidechain-Sidechain	108	17.5	98	90.7	15.9	75	69.4	12.2

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> 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 <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	402	161	4	22	0	589	2.96	4.7	1.0	2.93
2	402	161	4	22	0	589	2.91	4.71	1.09	2.88
3	402	161	4	22	0	589	2.91	4.72	1.02	2.86
4	401	150	4	22	0	577	2.91	6.76	1.06	2.83
5	402	161	4	22	0	589	2.89	4.71	1.04	2.84
6	401	162	4	22	0	589	2.91	4.71	1.06	2.9
7	402	159	1	22	0	584	2.91	4.83	1.0	2.86
8	402	160	4	22	0	588	2.92	4.72	1.05	2.88
9	402	162	4	22	0	590	2.96	4.67	0.95	2.97
10	402	164	4	22	0	592	2.95	4.71	0.99	2.87

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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	402	161	4	22	0	589	2.92	4.69	1.02	2.87
12	402	163	4	22	0	591	2.92	4.72	1.02	2.88
13	402	157	4	22	0	585	2.92	4.71	1.05	2.91
14	402	157	1	22	0	582	2.9	5.42	1.03	2.88
15	402	160	4	22	0	588	2.9	4.73	1.02	2.79
16	396	158	4	22	0	580	2.95	4.77	1.03	3.01
17	402	162	4	22	0	590	2.97	4.73	0.96	2.89
18	402	163	4	22	0	591	2.93	4.67	1.03	2.97
19	402	162	4	22	0	590	2.9	4.7	1.01	2.97
20	402	157	4	22	0	585	2.86	4.7	1.07	2.93
21	402	161	4	22	0	589	2.92	4.73	0.98	2.8
22	402	160	4	22	0	588	2.94	4.7	0.98	2.95
23	402	162	4	22	0	590	2.99	4.72	0.96	2.95
24	402	163	4	22	0	591	2.98	4.66	0.95	2.94
25	401	161	4	22	0	588	2.85	4.71	1.07	2.82
26	402	158	4	21	0	585	2.9	4.7	1.03	2.85
27	402	155	4	22	0	583	2.89	4.66	1.02	2.87
28	402	160	1	22	0	585	2.92	5.81	1.01	2.8
29	402	162	4	21	0	589	2.99	4.72	0.99	2.93
30	402	161	4	22	0	589	2.92	4.7	1.02	2.87
31	402	156	4	22	0	584	2.91	4.74	1.1	2.92
32	402	158	4	22	0	586	2.91	6.15	1.04	2.91
33	402	162	4	22	0	590	2.97	4.74	0.97	2.86
34	402	162	4	22	0	590	2.93	4.75	1.01	2.93
35	402	153	4	22	0	581	2.91	4.72	1.05	2.89
36	402	160	4	24	0	590	2.95	4.74	0.99	2.89
37	402	164	4	23	0	593	2.93	4.68	1.01	2.9
38	402	164	4	24	0	594	2.93	4.84	1.02	2.82
39	402	161	4	25	0	592	2.91	4.68	0.98	2.87
40	402	161	4	22	0	589	2.89	4.72	1.07	2.97
41	402	164	4	24	0	594	2.94	4.75	1.01	2.89
42	402	163	4	23	0	592	2.9	4.7	1.01	2.89
43	402	155	4	22	0	583	2.89	4.76	1.05	2.87
44	402	162	4	22	0	590	2.92	4.71	1.06	2.94
45	402	161	4	22	0	589	2.94	4.68	0.95	2.9
46	402	162	4	22	0	590	2.84	4.7	1.09	2.76
47	402	160	4	24	0	590	2.88	5.97	1.07	2.79
48	402	164	4	22	0	592	2.91	4.72	1.03	2.8
49	402	164	4	22	0	592	2.86	5.95	1.06	2.77
50	402	162	4	22	0	590	2.93	4.74	1.01	2.82
51	402	162	4	22	0	590	2.95	4.7	1.02	2.9

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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
52	402	160	4	22	0	588	2.88	4.7	1.03	2.86
53	402	161	4	22	0	589	2.94	4.75	1.0	2.89
54	402	162	4	23	0	591	2.88	4.67	1.07	2.82
55	399	160	4	22	0	585	2.87	4.76	1.12	2.93
56	402	162	4	22	0	590	2.9	4.73	1.04	2.94
57	402	163	4	22	0	591	2.88	5.84	1.07	2.9
58	402	158	4	22	0	586	2.95	4.74	0.99	2.91
59	402	159	4	25	0	590	2.85	7.87	1.07	2.84
60	402	159	4	22	0	587	2.87	4.71	1.04	2.84
61	402	159	3	22	0	586	2.88	4.75	1.04	2.89
62	402	164	4	21	0	591	2.85	4.72	1.06	2.77
63	402	161	4	22	0	589	2.84	4.71	1.11	2.85
64	401	153	4	22	0	580	2.92	4.73	1.04	2.86
65	402	164	4	22	0	592	2.88	5.76	1.06	2.83
66	400	164	4	22	0	590	2.95	4.71	1.03	2.9
67	402	162	4	22	0	590	2.95	4.74	0.98	2.91
68	402	158	4	22	0	586	2.91	4.7	1.01	2.84
69	402	163	4	24	0	593	2.88	5.89	1.08	2.86
70	402	156	4	21	0	583	2.92	4.74	1.02	2.93
71	402	163	4	22	0	591	2.96	4.74	0.99	2.92
72	402	161	4	22	0	589	2.89	4.67	1.03	2.79
73	402	162	4	22	0	590	2.91	4.73	1.03	2.9
74	402	157	4	23	0	586	2.9	4.71	1.01	2.84
75	402	161	4	22	0	589	3.0	4.71	0.97	2.93
76	402	163	4	23	0	592	2.92	4.73	1.01	2.83
77	402	164	4	22	0	592	2.92	4.75	1.02	2.86
78	402	161	4	22	0	589	2.93	4.74	0.98	2.84
79	400	160	4	21	0	585	2.87	4.7	1.06	2.92
80	402	159	4	25	0	590	2.92	8.19	1.02	2.89
81	402	161	1	22	0	586	2.89	5.5	1.04	2.82
82	402	160	4	22	0	588	2.93	4.66	1.01	2.86
83	402	163	4	22	0	591	2.91	5.7	1.08	2.91
84	402	161	4	22	0	589	2.91	4.74	1.01	2.8
85	402	160	4	24	0	590	2.92	4.7	1.02	2.87
86	402	160	4	22	0	588	2.96	4.75	0.97	2.88
87	400	158	4	22	0	584	2.84	4.7	1.07	2.72
88	402	161	4	22	0	589	2.98	4.67	0.97	2.94
89	402	163	4	22	0	591	2.93	4.68	1.01	2.84
90	402	155	4	22	0	583	2.95	4.78	0.97	2.84
91	402	161	4	22	0	589	2.95	4.73	1.0	2.9
92	402	163	4	22	0	591	2.98	5.45	0.99	3.03

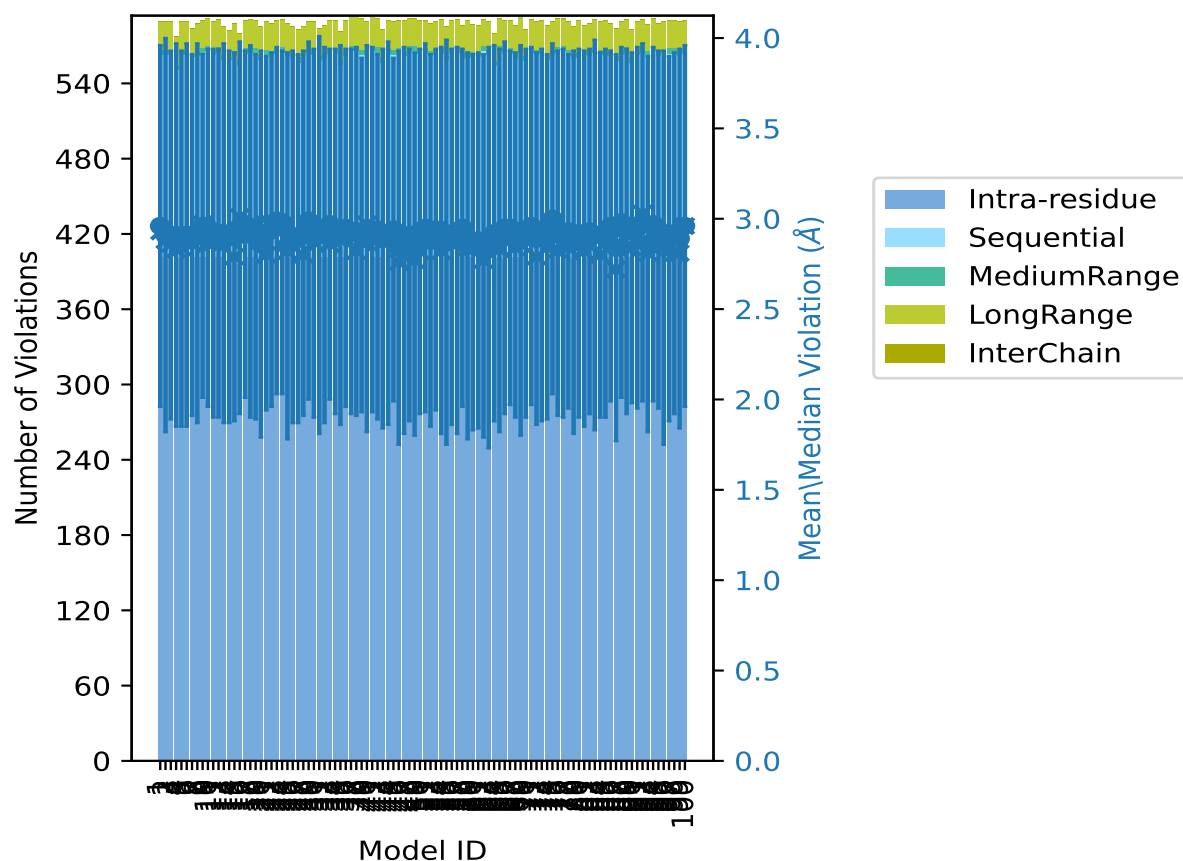
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
93	402	161	3	21	0	587	2.86	4.72	1.04	2.81
94	402	164	4	22	0	592	2.97	4.7	0.98	2.92
95	402	160	4	22	0	588	2.94	4.75	0.99	2.9
96	402	162	3	22	0	589	2.84	4.75	1.09	2.91
97	402	162	4	22	0	590	2.89	4.74	1.01	2.84
98	402	162	4	22	0	590	2.92	4.7	1.0	2.81
99	402	160	4	23	0	589	2.89	4.72	1.05	2.81
100	402	162	4	22	0	590	2.96	4.68	1.0	2.96

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard 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, 0(IR:0, SQ:0, MR:0, LR:0, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	0	0	0	0	0	1	1.0
0	0	0	0	0	0	2	2.0
0	0	0	0	0	0	3	3.0
0	0	0	0	0	0	4	4.0
0	0	0	0	0	0	5	5.0
0	0	0	0	0	0	6	6.0
0	0	0	0	0	0	7	7.0
0	0	0	0	0	0	8	8.0
0	0	0	0	0	0	9	9.0
0	0	0	0	0	0	10	10.0
0	0	0	0	0	0	11	11.0
0	0	0	0	0	0	12	12.0
0	0	0	0	0	0	13	13.0
0	0	0	0	0	0	14	14.0
0	0	0	0	0	0	15	15.0
0	0	0	0	0	0	16	16.0
0	0	0	0	0	0	17	17.0
0	0	0	0	0	0	18	18.0
0	0	0	0	0	0	19	19.0
0	0	0	0	0	0	20	20.0
0	0	0	0	0	0	21	21.0
0	0	0	0	0	0	22	22.0
0	0	0	0	0	0	23	23.0
0	0	0	0	0	0	24	24.0
0	0	0	0	0	0	25	25.0
0	0	0	0	0	0	26	26.0
0	0	0	0	0	0	27	27.0
0	0	0	0	0	0	28	28.0
0	0	0	0	0	0	29	29.0
0	0	0	0	0	0	30	30.0
0	0	0	0	0	0	31	31.0
0	0	0	0	0	0	32	32.0
0	0	0	0	0	0	33	33.0
0	0	0	0	0	0	34	34.0
0	0	0	0	0	0	35	35.0
0	0	0	0	0	0	36	36.0

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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	0	0	0	0	0	37	37.0
0	0	0	0	0	0	38	38.0
0	1	0	0	0	1	39	39.0
0	0	0	0	0	0	40	40.0
0	0	0	0	0	0	41	41.0
0	0	0	0	0	0	42	42.0
0	0	0	0	0	0	43	43.0
0	0	0	0	0	0	44	44.0
0	0	0	0	0	0	45	45.0
0	0	0	0	0	0	46	46.0
0	0	0	0	0	0	47	47.0
0	0	0	0	0	0	48	48.0
0	0	0	0	0	0	49	49.0
0	0	0	0	0	0	50	50.0
0	0	0	0	0	0	51	51.0
0	0	0	0	0	0	52	52.0
0	0	0	0	0	0	53	53.0
0	0	0	0	0	0	54	54.0
0	0	0	0	0	0	55	55.0
0	0	0	0	0	0	56	56.0
0	0	0	0	0	0	57	57.0
0	0	0	0	0	0	58	58.0
0	0	0	0	0	0	59	59.0
0	0	0	0	0	0	60	60.0
0	0	0	0	0	0	61	61.0
0	0	0	0	0	0	62	62.0
0	0	0	0	0	0	63	63.0
0	0	0	0	0	0	64	64.0
0	0	0	0	0	0	65	65.0
0	0	0	0	0	0	66	66.0
0	0	0	0	0	0	67	67.0
0	0	0	0	0	0	68	68.0
0	0	0	0	0	0	69	69.0
0	0	0	0	0	0	70	70.0
0	0	0	0	0	0	71	71.0
0	1	0	0	0	1	72	72.0
0	0	0	0	0	0	73	73.0
0	0	0	0	0	0	74	74.0
0	0	0	0	0	0	75	75.0
0	0	0	0	0	0	76	76.0
0	0	0	0	0	0	77	77.0

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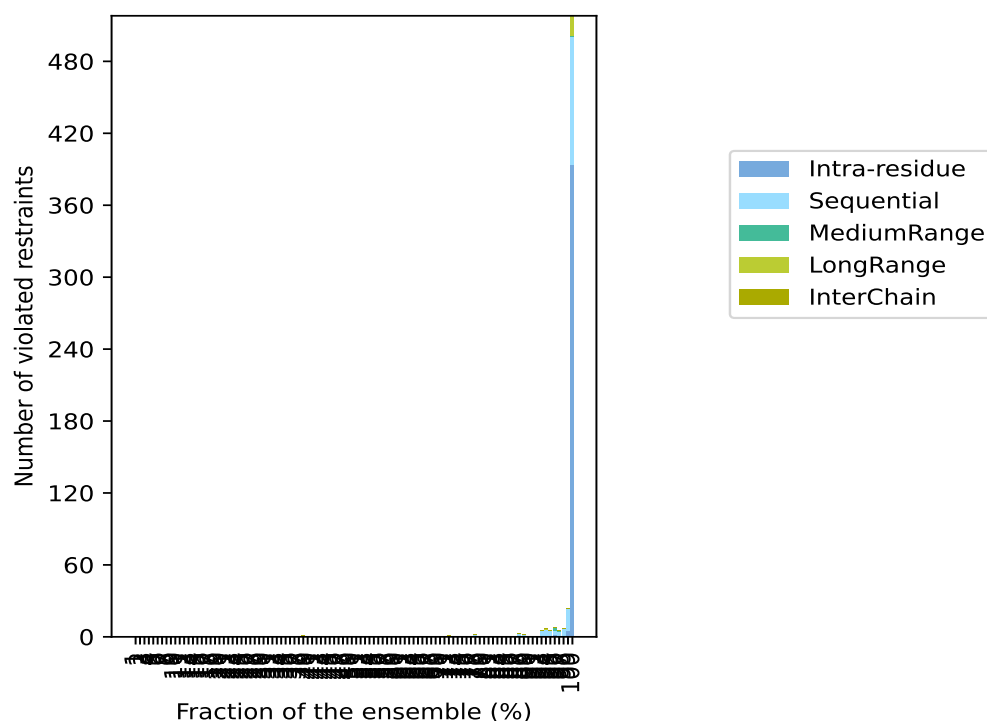
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	2	0	0	0	2	78	78.0
0	0	0	0	0	0	79	79.0
0	0	0	0	0	0	80	80.0
0	0	0	0	0	0	81	81.0
0	0	0	0	0	0	82	82.0
0	0	0	0	0	0	83	83.0
0	0	0	0	0	0	84	84.0
0	0	0	0	0	0	85	85.0
0	0	0	0	0	0	86	86.0
0	0	0	0	0	0	87	87.0
0	3	0	0	0	3	88	88.0
0	2	0	0	0	2	89	89.0
0	0	0	0	0	0	90	90.0
0	0	0	0	0	0	91	91.0
0	0	0	0	0	0	92	92.0
0	5	0	0	0	5	93	93.0
1	5	0	1	0	7	94	94.0
0	5	0	0	0	5	95	95.0
2	3	3	0	0	8	96	96.0
0	4	1	0	0	5	97	97.0
0	7	0	0	0	7	98	98.0
5	19	0	0	0	24	99	99.0
394	107	0	17	0	518	100	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

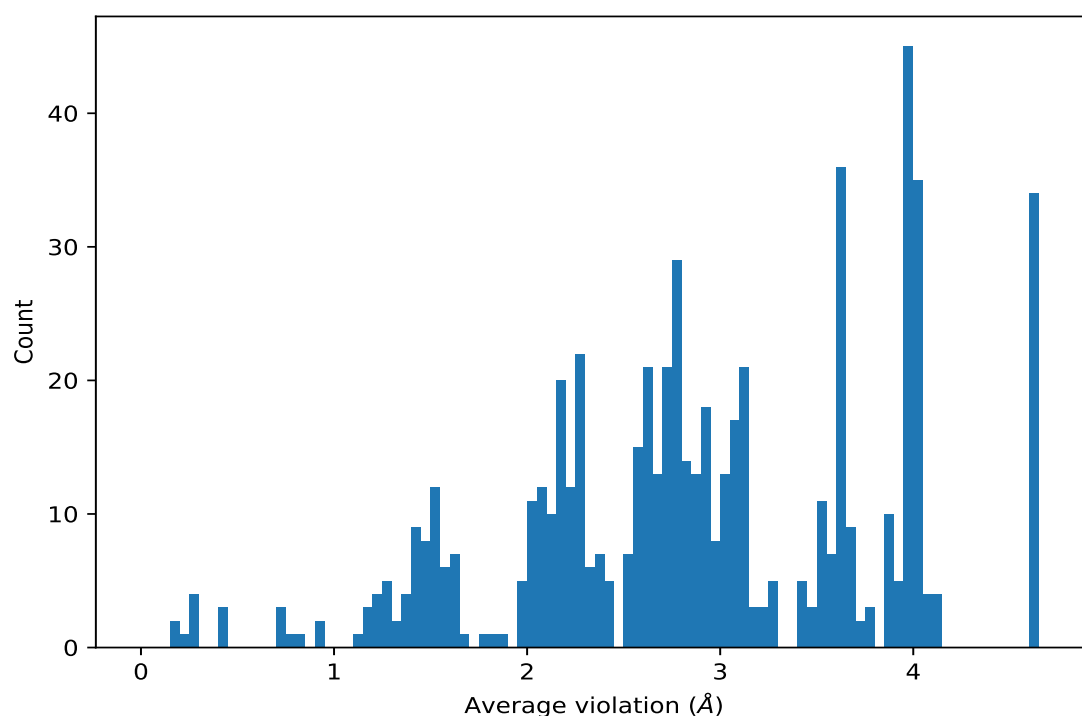
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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 <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,103)	1:10:A:G:H5''	1:10:A:G:H5'	100	4.64	0.05	4.64
(1,77)	1:7:A:C:H5''	1:7:A:C:H5'	100	4.64	0.05	4.64
(2,67)	1:7:A:C:H5''	1:7:A:C:H5'	100	4.64	0.05	4.64
(3,65)	1:7:A:C:H5''	1:7:A:C:H5'	100	4.64	0.05	4.64
(4,52)	1:7:A:C:H5''	1:7:A:C:H5'	100	4.64	0.05	4.64
(5,57)	1:7:A:C:H5''	1:7:A:C:H5'	100	4.64	0.05	4.64
(1,37)	1:4:A:A:H5''	1:4:A:A:H5'	100	4.64	0.05	4.63
(2,21)	1:3:A:C:H42	1:3:A:C:H41	100	4.64	0.03	4.64
(4,17)	1:3:A:C:H42	1:3:A:C:H41	100	4.64	0.03	4.64
(2,120)	1:14:A:C:H42	1:14:A:C:H41	100	4.64	0.04	4.63

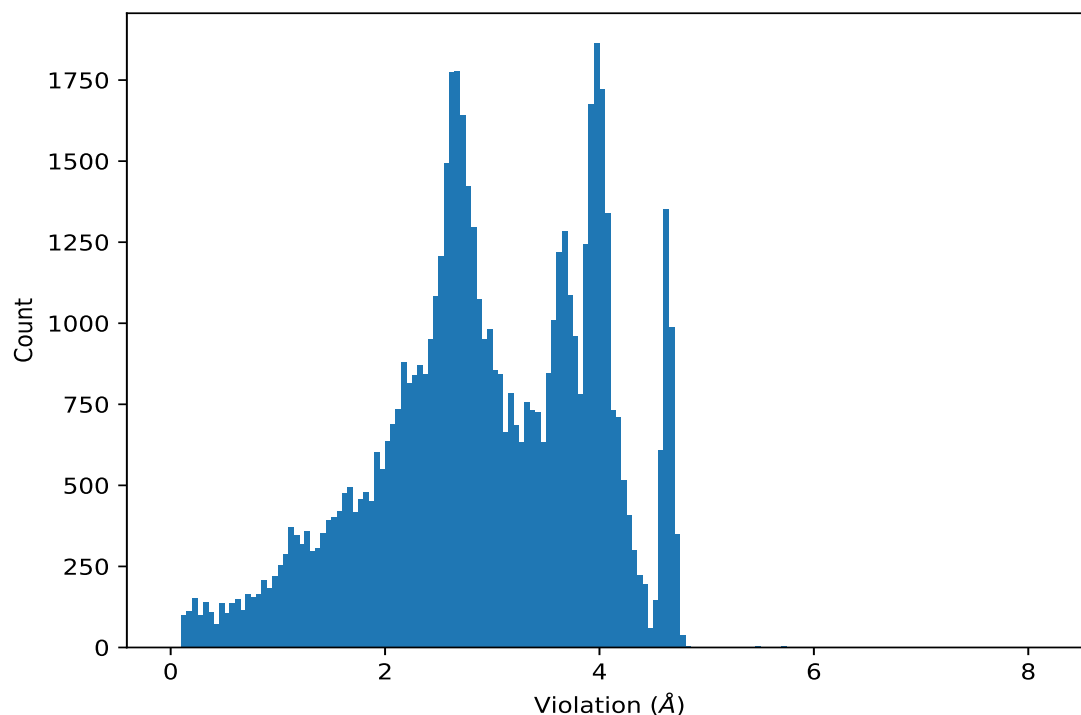
<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation



## 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)
(6,6)	1:14:A:C:O2	1:1:A:G:H22	80	8.19
(2,53)	1:6:A:G:H1'	1:10:A:G:H1	59	7.87
(1,82)	1:8:A:A:H1'	1:9:A:A:H2	4	6.76
(6,5)	1:14:A:C:O2	1:1:A:G:N2	80	6.29
(2,53)	1:6:A:G:H1'	1:10:A:G:H1	32	6.15
(2,53)	1:6:A:G:H1'	1:10:A:G:H1	47	5.97
(2,53)	1:6:A:G:H1'	1:10:A:G:H1	49	5.95
(2,53)	1:6:A:G:H1'	1:10:A:G:H1	69	5.89
(2,53)	1:6:A:G:H1'	1:10:A:G:H1	57	5.84
(2,53)	1:6:A:G:H1'	1:10:A:G:H1	28	5.81

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found