



wwPDB NMR Structure Validation Summary Report ⓘ

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BMRB ID : 17601
Title : Solution structure of the MLV readthrough pseudoknot
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Deposited on : 2011-04-26

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

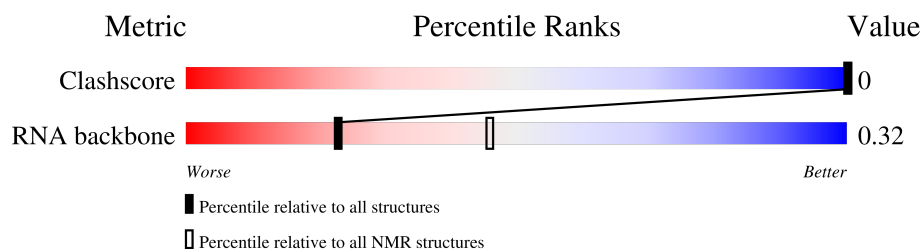
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 21%.

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	63	 79% 10% 11%

2 Ensemble composition and analysis ⓘ

This entry contains 10 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](#)

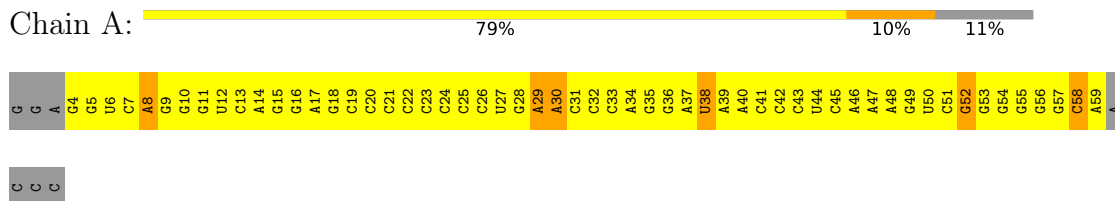
There is only 1 type of molecule in this entry. The entry contains 1810 atoms, of which 610 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called RNA (56-MER).

Mol	Chain	Residues	Atoms						Trace
1	A	56	Total	C	H	N	O	P	0
			1810	535	610	224	385	56	

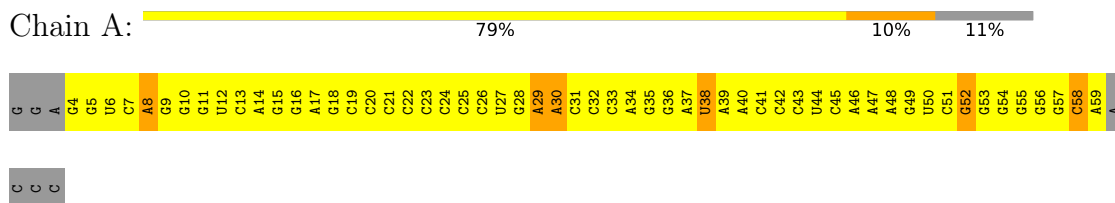
4.1 Average score per residue in the NMR ensemble

- Molecule 1: RNA (56-MER)



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

- Molecule 1: RNA (56-MER)



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	274
Number of shifts mapped to atoms	240
Number of unparsed shifts	0
Number of shifts with mapping errors	34
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	21%

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	0.66±0.00	0±0/1342 (0.0± 0.0%)	2.58±0.02	217±3/2091 (10.4± 0.1%)
All	All	0.66	0/13420 (0.0%)	2.58	2168/20910 (10.4%)

There are no bond-length outliers.

5 of 227 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	38	U	O4'-C4'-C3'	-13.87	90.13	104.00	8	6
1	A	44	U	O4'-C4'-C3'	-13.79	90.20	104.00	3	10
1	A	45	C	O4'-C4'-C3'	-13.78	90.22	104.00	6	10
1	A	48	A	O4'-C4'-C3'	-13.72	90.28	104.00	4	10
1	A	51	C	O4'-C4'-C3'	-13.61	90.39	104.00	8	10

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
All	All	12000	6100	6110	-

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 -.

There are no clashes.

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	55/63 (87%)	6±0 (11±0%)	0±1 (1±1%)	0.38±0.00
All	All	550/630 (87%)	60 (11%)	5 (1%)	0.38

The overall RNA backbone suiteness is 0.32.

5 of 6 unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	8	A	10
1	A	29	A	10
1	A	30	A	10
1	A	38	U	10
1	A	52	G	10

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	38	U	4
1	A	49	G	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

The completeness of assignment taking into account all chemical shift lists is 21% for the well-defined parts and 21% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	274
Number of shifts mapped to atoms	240
Number of unparsed shifts	0
Number of shifts with mapping errors	34
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	84

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 34) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	G	H8	8.054	.	1
1	A	1	G	C8	117.296	.	1
1	A	2	G	H8	7.96	.	1
1	A	2	G	C8	115.882	.	1
1	A	3	A	H1'	6.0142	.	1
1	A	3	A	H2	7.728	.	1
1	A	3	A	H2'	4.7864	.	1
1	A	3	A	H8	8.0139	.	1
1	A	3	A	C1'	127.237	.	1
1	A	3	A	C2	130.975	.	1
1	A	3	A	C8	117.652	.	1
1	A	60	A	H1'	5.3783	.	1
1	A	60	A	H2	7.9054	.	1
1	A	60	A	H2'	4.3098	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	60	A	H8	7.644	.	1
1	A	60	A	C1'	109.859	.	1
1	A	60	A	C2	112.439	.	1
1	A	60	A	C8	116.36	.	1
1	A	61	C	H1'	5.1863	.	1
1	A	61	C	H2'	4.0636	.	1
1	A	61	C	H5	5.1428	.	1
1	A	61	C	H6	7.1889	.	1
1	A	61	C	C1'	110.809	.	1
1	A	61	C	C5	114.706	.	1
1	A	62	C	H1'	5.5783	.	1
1	A	62	C	H2'	4.1418	.	1
1	A	62	C	H5	5.637	.	1
1	A	62	C	H6	7.6443	.	1
1	A	62	C	C1'	118.952	.	1
1	A	62	C	C5	116.065	.	1
1	A	63	C	H1'	5.779	.	1
1	A	63	C	H5	5.8354	.	1
1	A	63	C	H6	7.7884	.	1
1	A	63	C	C5	116.375	.	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 21%, i.e. 228 atoms were assigned a chemical shift out of a possible 1070. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Sugar	68/616 (11%)	54/336 (16%)	14/280 (5%)	0/0 (—%)
Base	160/454 (35%)	101/286 (35%)	59/94 (63%)	0/74 (0%)
Overall	228/1070 (21%)	155/622 (25%)	73/374 (20%)	0/74 (0%)

7.1.4 Statistically unusual chemical shifts ⓘ

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	14	A	C1'	130.38	82.09 – 100.58	21.1
1	A	34	A	C1'	129.45	82.09 – 100.58	20.6
1	A	48	A	C1'	128.43	82.09 – 100.58	20.1
1	A	38	U	C6	100.14	131.00 – 152.02	-19.7
1	A	14	A	C2	109.71	142.12 – 164.22	-19.7
1	A	12	U	C6	100.30	131.00 – 152.02	-19.6
1	A	50	U	C6	100.52	131.00 – 152.02	-19.5
1	A	6	U	C6	100.55	131.00 – 152.02	-19.5
1	A	27	U	C6	100.60	131.00 – 152.02	-19.5
1	A	3	A	C1'	127.24	82.09 – 100.58	19.4
1	A	59	A	C2	110.95	142.12 – 164.22	-19.1
1	A	37	A	C2	111.80	142.12 – 164.22	-18.7
1	A	30	A	C2	111.86	142.12 – 164.22	-18.7
1	A	34	A	C2	112.10	142.12 – 164.22	-18.6
1	A	47	A	C2	112.28	142.12 – 164.22	-18.5
1	A	46	A	C2	112.33	142.12 – 164.22	-18.5
1	A	60	A	C2	112.44	142.12 – 164.22	-18.4
1	A	48	A	C2	112.55	142.12 – 164.22	-18.4
1	A	17	A	C2	112.89	142.12 – 164.22	-18.2
1	A	62	C	C1'	118.95	83.64 – 101.51	14.8
1	A	58	C	C6	117.60	132.94 – 149.05	-14.5
1	A	24	C	C6	117.96	132.94 – 149.05	-14.3
1	A	31	C	C6	118.78	132.94 – 149.05	-13.8
1	A	42	C	C5	116.40	89.67 – 104.57	12.9
1	A	63	C	C5	116.38	89.67 – 104.57	12.9
1	A	41	C	C5	116.31	89.67 – 104.57	12.9
1	A	62	C	C5	116.06	89.67 – 104.57	12.7
1	A	45	C	C5	115.92	89.67 – 104.57	12.6
1	A	25	C	C5	115.35	89.67 – 104.57	12.2
1	A	26	C	C5	115.29	89.67 – 104.57	12.2
1	A	51	C	C5	115.08	89.67 – 104.57	12.1
1	A	61	C	C5	114.71	89.67 – 104.57	11.8
1	A	31	C	C5	114.65	89.67 – 104.57	11.8
1	A	60	A	C8	116.36	129.50 – 149.86	-11.5
1	A	34	A	C8	116.95	129.50 – 149.86	-11.2
1	A	59	A	C8	117.06	129.50 – 149.86	-11.1
1	A	3	A	C8	117.65	129.50 – 149.86	-10.8
1	A	11	G	C8	112.85	125.77 – 148.14	-10.8

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	56	G	C8	112.85	125.77 – 148.14	-10.8
1	A	57	G	C8	112.85	125.77 – 148.14	-10.8
1	A	8	A	C8	117.84	129.50 – 149.86	-10.7
1	A	37	A	C8	117.84	129.50 – 149.86	-10.7
1	A	36	G	C8	113.07	125.77 – 148.14	-10.7
1	A	55	G	C8	113.06	125.77 – 148.14	-10.7
1	A	10	G	C8	113.25	125.77 – 148.14	-10.6
1	A	35	G	C8	113.37	125.77 – 148.14	-10.5
1	A	48	A	C8	118.26	129.50 – 149.86	-10.5
1	A	4	G	C8	113.41	125.77 – 148.14	-10.5
1	A	15	G	C8	113.46	125.77 – 148.14	-10.5
1	A	59	A	C1'	110.74	82.09 – 100.58	10.5
1	A	40	A	C8	118.63	129.50 – 149.86	-10.3
1	A	47	A	C8	118.67	129.50 – 149.86	-10.3
1	A	30	A	C8	118.69	129.50 – 149.86	-10.3
1	A	54	G	C8	114.03	125.77 – 148.14	-10.2
1	A	5	G	C8	114.07	125.77 – 148.14	-10.2
1	A	9	G	C8	114.09	125.77 – 148.14	-10.2
1	A	61	C	C1'	110.81	83.64 – 101.51	10.2
1	A	16	G	C8	114.13	125.77 – 148.14	-10.2
1	A	29	A	C8	118.91	129.50 – 149.86	-10.2
1	A	46	A	C8	119.02	129.50 – 149.86	-10.2
1	A	39	A	C8	119.14	129.50 – 149.86	-10.1
1	A	53	G	C8	114.42	125.77 – 148.14	-10.1
1	A	3	A	C2	130.97	142.12 – 164.22	-10.0
1	A	30	A	C1'	109.88	82.09 – 100.58	10.0
1	A	60	A	C1'	109.86	82.09 – 100.58	10.0
1	A	17	A	C8	119.87	129.50 – 149.86	-9.7
1	A	28	G	C8	115.24	125.77 – 148.14	-9.7
1	A	8	A	C1'	108.90	82.09 – 100.58	9.5
1	A	52	G	C8	115.75	125.77 – 148.14	-9.5
1	A	39	A	C2	132.32	142.12 – 164.22	-9.4
1	A	2	G	C8	115.88	125.77 – 148.14	-9.4
1	A	8	A	C2	132.39	142.12 – 164.22	-9.4
1	A	40	A	C2	132.59	142.12 – 164.22	-9.3
1	A	47	A	C1'	108.46	82.09 – 100.58	9.3
1	A	29	A	C2	132.72	142.12 – 164.22	-9.2
1	A	18	G	C8	116.31	125.77 – 148.14	-9.2
1	A	42	C	C1'	109.03	83.64 – 101.51	9.2
1	A	49	G	C8	116.61	125.77 – 148.14	-9.1
1	A	46	A	C1'	107.99	82.09 – 100.58	9.0
1	A	29	A	C1'	107.94	82.09 – 100.58	9.0

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List Id	Chain	Res	Type	Atom	Shift, <i>ppm</i>	Expected range, <i>ppm</i>	Z-score
1	A	40	A	C1'	107.92	82.09 – 100.58	9.0
1	A	39	A	C1'	107.61	82.09 – 100.58	8.8
1	A	1	G	C8	117.30	125.77 – 148.14	-8.8
1	A	17	A	C1'	106.01	82.09 – 100.58	7.9

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	980
Intra-residue ($ i-j =0$)	574
Sequential ($ i-j =1$)	113
Medium range ($ i-j >1$ and $ i-j <5$)	4
Long range ($ i-j \geq 5$)	190
Inter-chain	0
Hydrogen bond restraints	99
Disulfide bond restraints	0
Total dihedral-angle restraints	281
Number of unmapped restraints	0
Number of restraints per residue	20.0
Number of long range restraints per residue ¹	4.6

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)	None	None
0.2-0.5 (Medium)	None	None
>0.5 (Large)	48.0	4.32

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	0.1	1.57
10.0-20.0 (Medium)	0.4	14.43
>20.0 (Large)	0.7	38.06

9 Distance violation analysis ⓘ

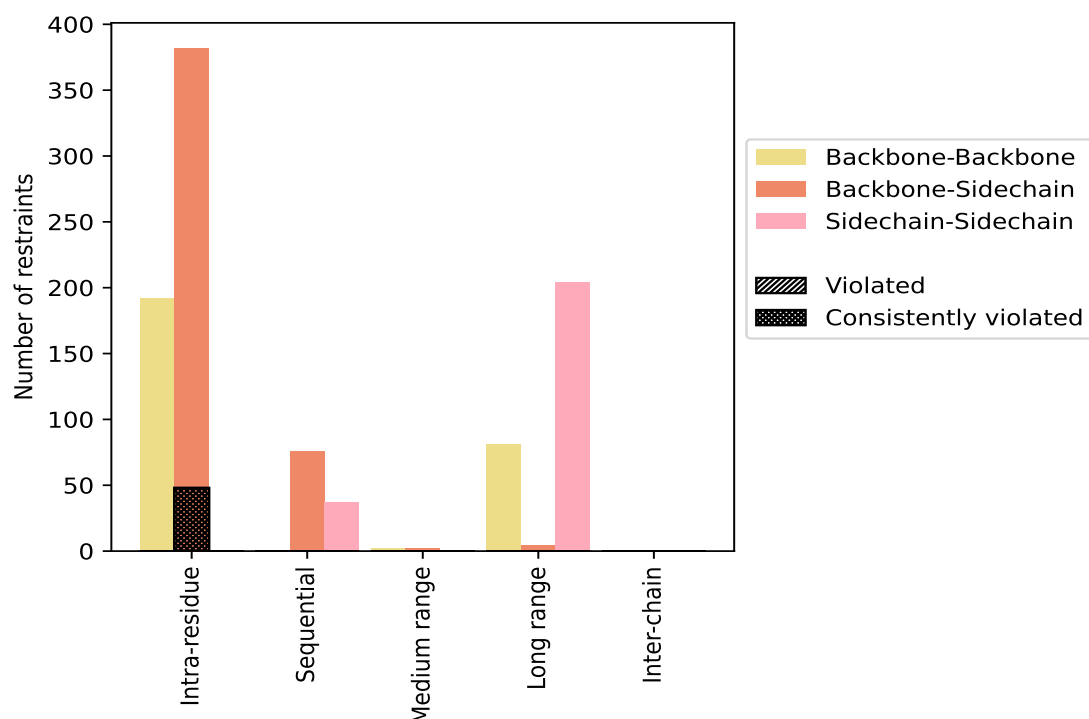
9.1 Summary of distance violations ⓘ

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)	574	58.6	48	8.4	4.9	48	8.4	4.9
Backbone-Backbone	192	19.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	382	39.0	48	12.6	4.9	48	12.6	4.9
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	113	11.5	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	76	7.8	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	37	3.8	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	4	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	2	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2	0.2	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
Long range (i-j ≥5)	190	19.4	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	81	8.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	4	0.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	105	10.7	0	0.0	0.0	0	0.0	0.0
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	99	10.1	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	980	100.0	48	4.9	4.9	48	4.9	4.9
Backbone-Backbone	275	28.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	464	47.3	48	10.3	4.9	48	10.3	4.9
Sidechain-Sidechain	241	24.6	0	0.0	0.0	0	0.0	0.0

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

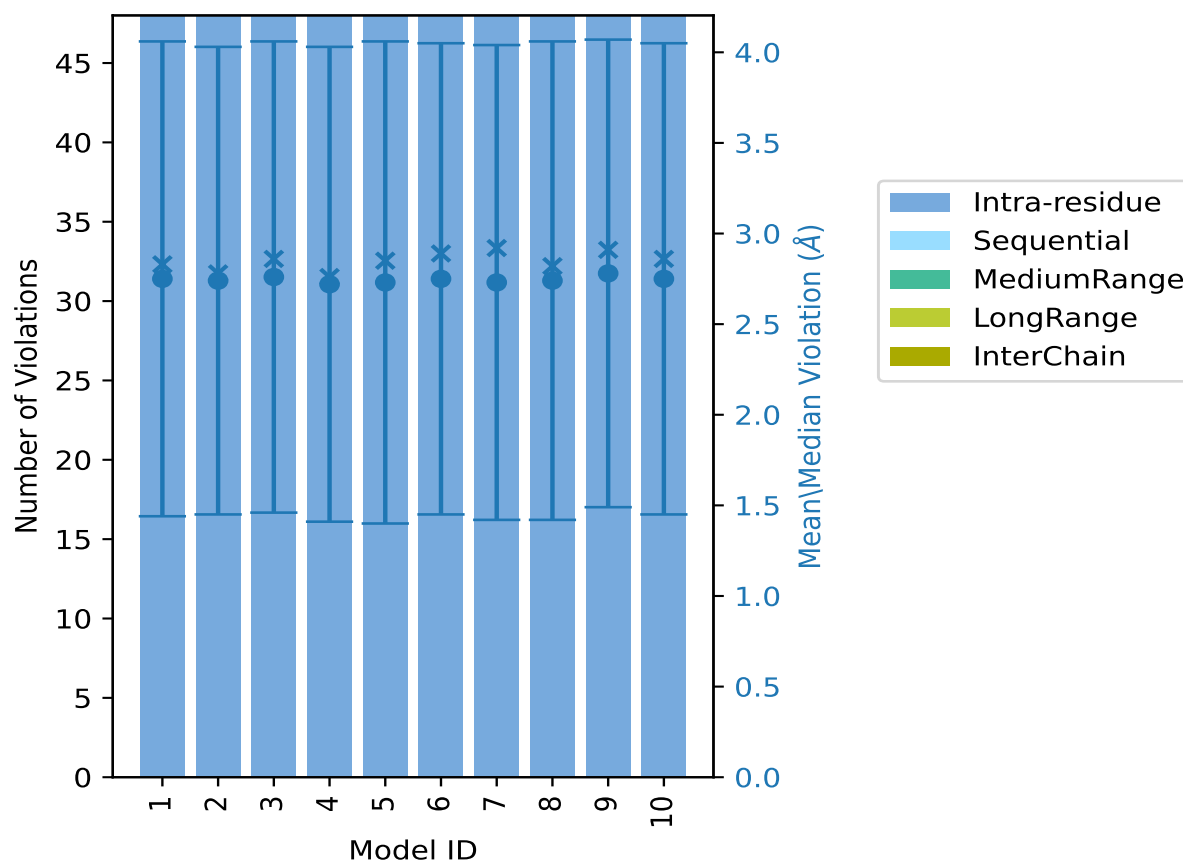
9.2 Distance violation statistics for each model [i](#)

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	48	0	0	0	0	48	2.75	4.23	1.31	2.83
2	48	0	0	0	0	48	2.74	4.23	1.29	2.78
3	48	0	0	0	0	48	2.76	4.28	1.3	2.86
4	48	0	0	0	0	48	2.72	4.16	1.31	2.76
5	48	0	0	0	0	48	2.73	4.28	1.33	2.85
6	48	0	0	0	0	48	2.75	4.32	1.3	2.89
7	48	0	0	0	0	48	2.73	4.3	1.31	2.92
8	48	0	0	0	0	48	2.74	4.28	1.32	2.82
9	48	0	0	0	0	48	2.78	4.29	1.29	2.91
10	48	0	0	0	0	48	2.75	4.26	1.3	2.86

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



The mean(dot), median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 833(IR:526, SQ:113, MR:4, LR:190, 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	0	0	0	0	0	1	10.0
0	0	0	0	0	0	2	20.0
0	0	0	0	0	0	3	30.0

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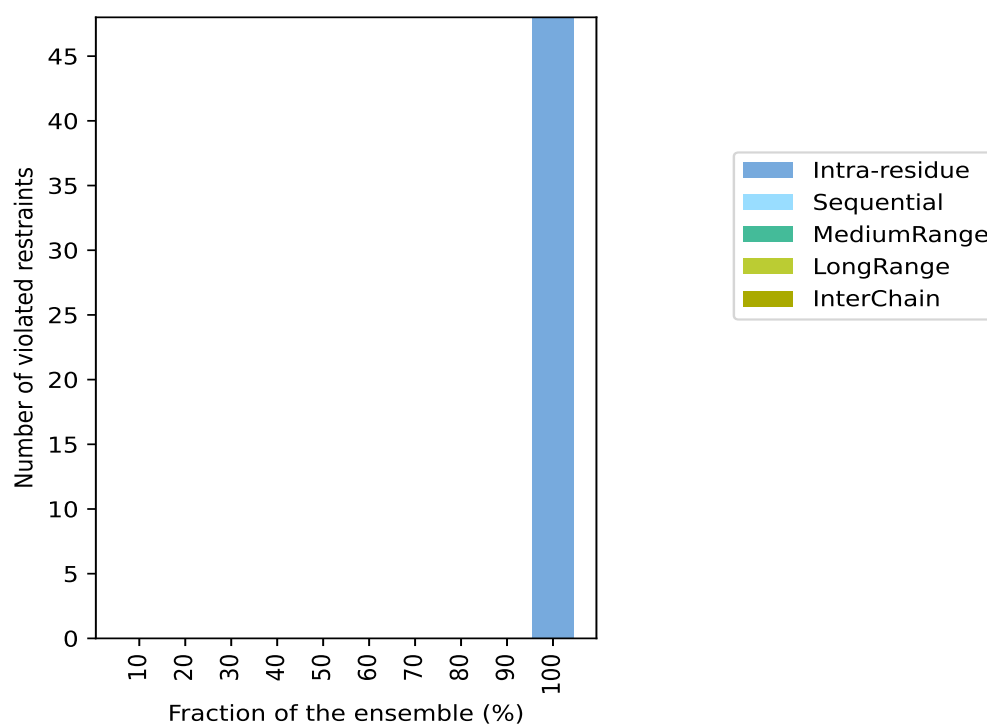
Continued from previous page...

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	4	40.0
0	0	0	0	0	0	5	50.0
0	0	0	0	0	0	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	0	0	0	8	80.0
0	0	0	0	0	0	9	90.0
48	0	0	0	0	48	10	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 ⓘ

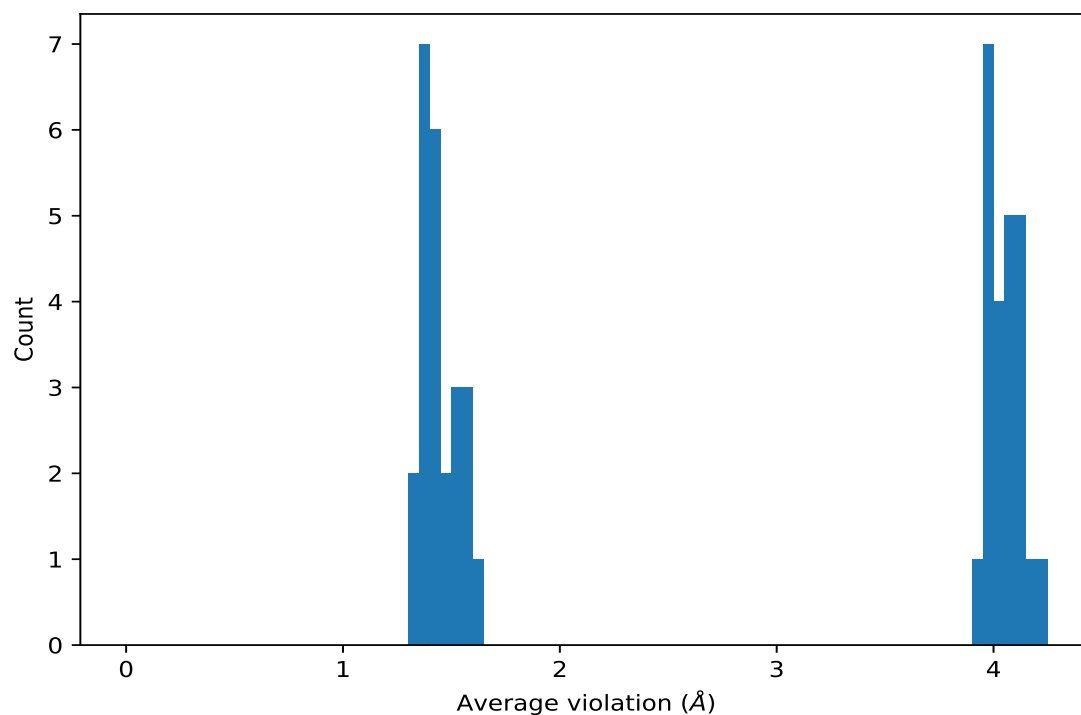


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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.

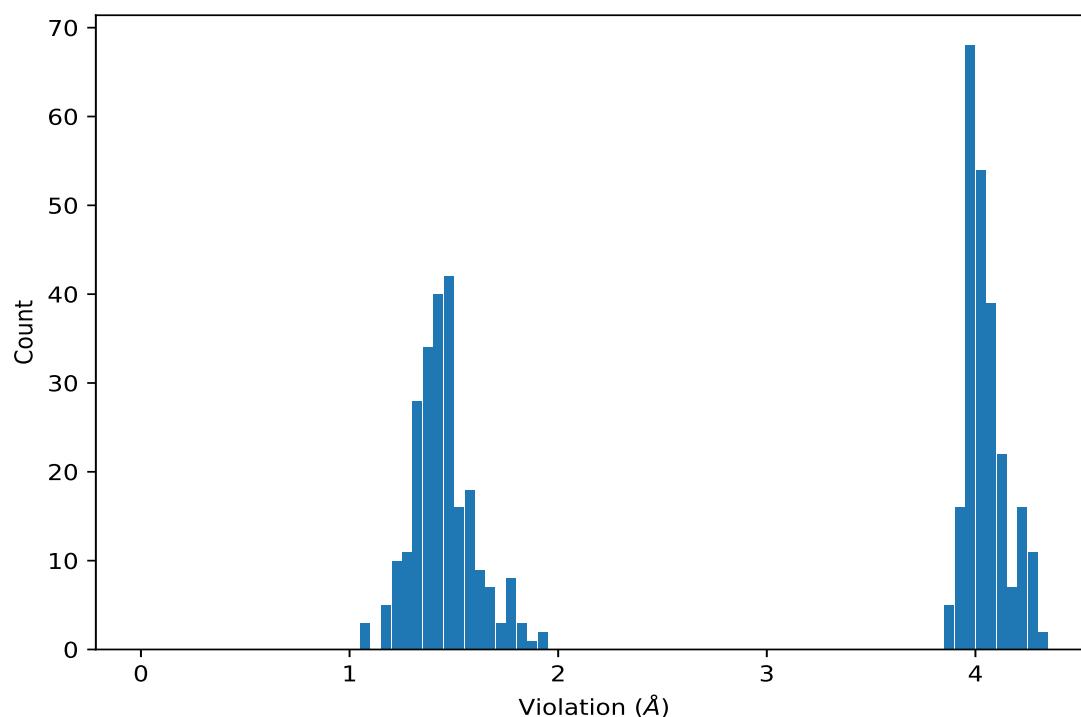
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,429)	1:41:A:C:H4'	1:41:A:C:H5	10	4.2	0.08	4.2
(2,475)	1:51:A:C:H4'	1:51:A:C:H5	10	4.16	0.09	4.18
(2,439)	1:43:A:C:H4'	1:43:A:C:H5	10	4.14	0.09	4.18
(2,449)	1:45:A:C:H4'	1:45:A:C:H5	10	4.14	0.11	4.1
(2,470)	1:50:A:U:H4'	1:50:A:U:H5	10	4.11	0.08	4.1
(2,434)	1:42:A:C:H4'	1:42:A:C:H5	10	4.11	0.07	4.08
(2,444)	1:44:A:U:H4'	1:44:A:U:H5	10	4.11	0.12	4.03
(2,330)	1:25:A:C:H4'	1:25:A:C:H5	10	4.1	0.02	4.11
(2,230)	1:12:A:U:H4'	1:12:A:U:H5	10	4.09	0.08	4.08
(2,192)	1:7:A:C:H4'	1:7:A:C:H5	10	4.05	0.08	4.01

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)
(2,449)	1:45:A:C:H4'	1:45:A:C:H5	6	4.32
(2,429)	1:41:A:C:H4'	1:41:A:C:H5	7	4.3
(2,444)	1:44:A:U:H4'	1:44:A:U:H5	9	4.29
(2,475)	1:51:A:C:H4'	1:51:A:C:H5	3	4.28
(2,449)	1:45:A:C:H4'	1:45:A:C:H5	5	4.28
(2,429)	1:41:A:C:H4'	1:41:A:C:H5	5	4.28
(2,429)	1:41:A:C:H4'	1:41:A:C:H5	8	4.28
(2,475)	1:51:A:C:H4'	1:51:A:C:H5	8	4.27
(2,444)	1:44:A:U:H4'	1:44:A:U:H5	6	4.27
(2,470)	1:50:A:U:H4'	1:50:A:U:H5	5	4.26

10 Dihedral-angle violation analysis [i](#)

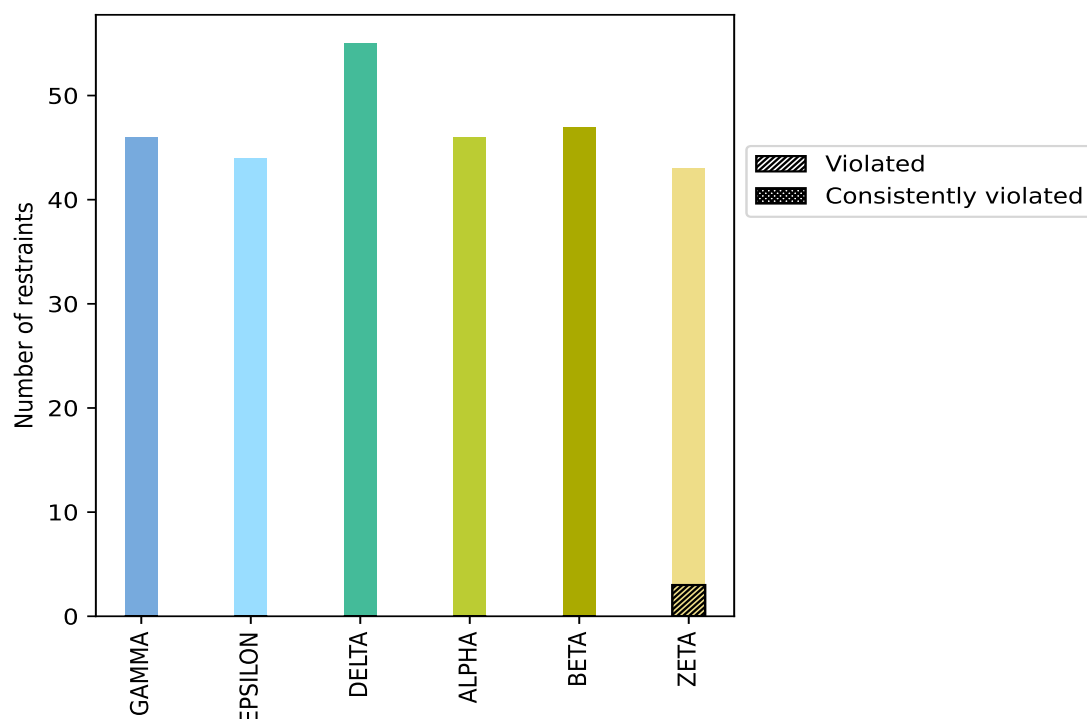
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
GAMMA	46	16.4	0	0.0	0.0	0	0.0	0.0
EPSILON	44	15.7	0	0.0	0.0	0	0.0	0.0
DELTA	55	19.6	0	0.0	0.0	0	0.0	0.0
ALPHA	46	16.4	0	0.0	0.0	0	0.0	0.0
BETA	47	16.7	0	0.0	0.0	0	0.0	0.0
ZETA	43	15.3	3	7.0	1.1	0	0.0	0.0
Total	281	100.0	3	1.1	1.1	0	0.0	0.0

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their

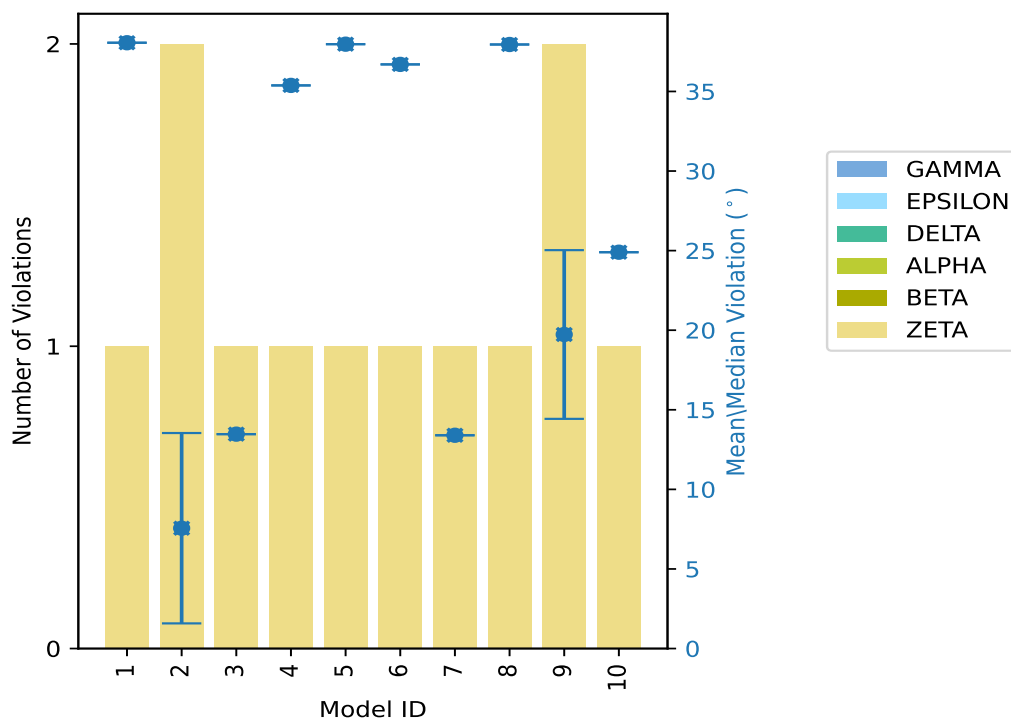
respective categories

10.2 Dihedral-angle violation statistics for each model [i](#)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations							Mean (°)	Max (°)
	GAMMA	EPSILON	DELTA	ALPHA	BETA	ZETA	Total		
1	0	0	0	0	0	1	1	38.06	38.06
2	0	0	0	0	0	2	2	7.56	13.54
3	0	0	0	0	0	1	1	13.47	13.47
4	0	0	0	0	0	1	1	35.38	35.38
5	0	0	0	0	0	1	1	37.97	37.97
6	0	0	0	0	0	1	1	36.7	36.7
7	0	0	0	0	0	1	1	13.4	13.4
8	0	0	0	0	0	1	1	37.95	37.95
9	0	0	0	0	0	2	2	19.73	25.02
10	0	0	0	0	0	1	1	24.9	24.9

10.2.1 Bar graph : Dihedral 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

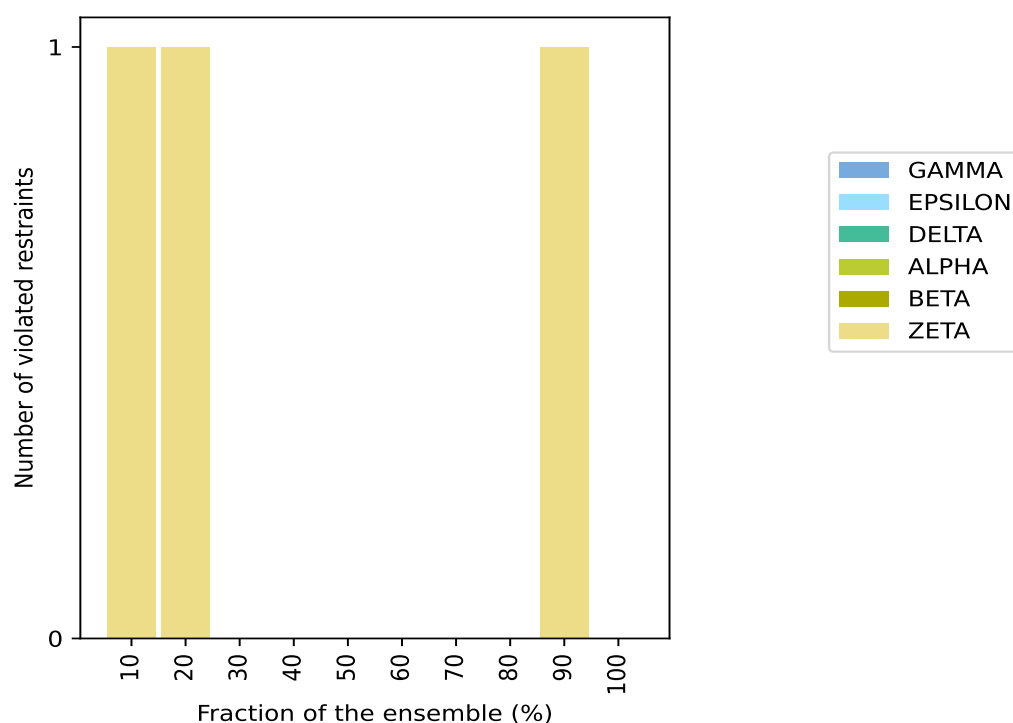
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints							Fraction of the ensemble	
GAMMA	EPSILON	DELTA	ALPHA	BETA	ZETA	Total	Count ¹	%
0	0	0	0	0	1	1	1	10.0
0	0	0	0	0	1	1	2	20.0
0	0	0	0	0	0	0	3	30.0
0	0	0	0	0	0	0	4	40.0
0	0	0	0	0	0	0	5	50.0
0	0	0	0	0	0	0	6	60.0
0	0	0	0	0	0	0	7	70.0
0	0	0	0	0	0	0	8	80.0
0	0	0	0	0	1	1	9	90.0
0	0	0	0	0	0	0	10	100.0

¹ Number of models with violations

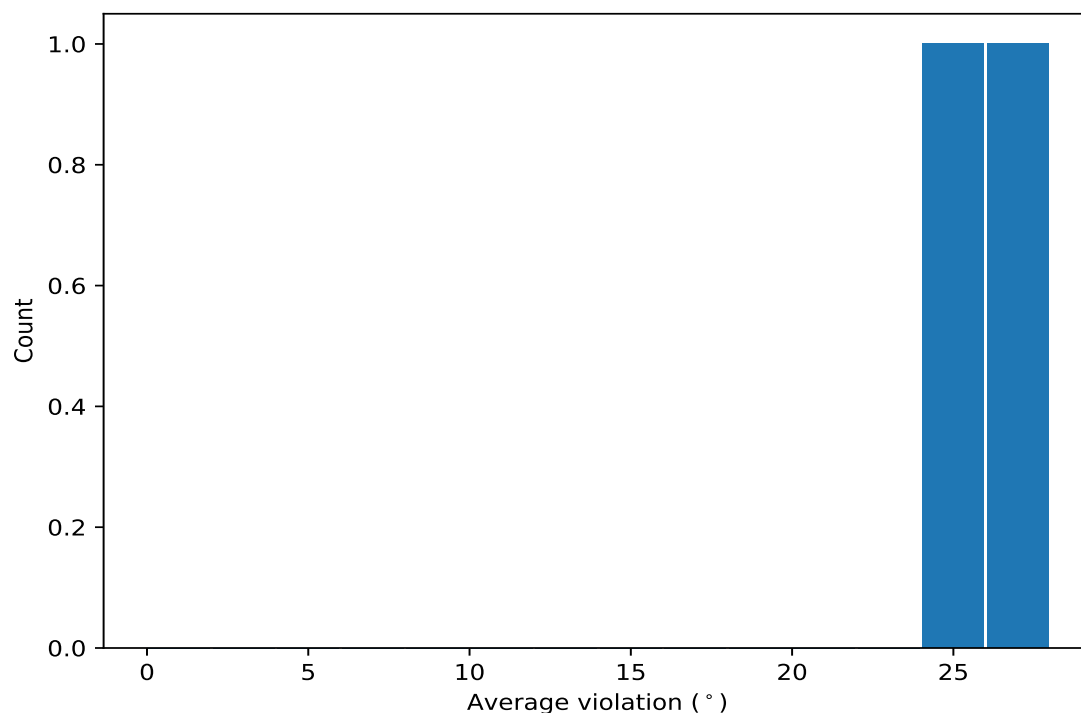
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

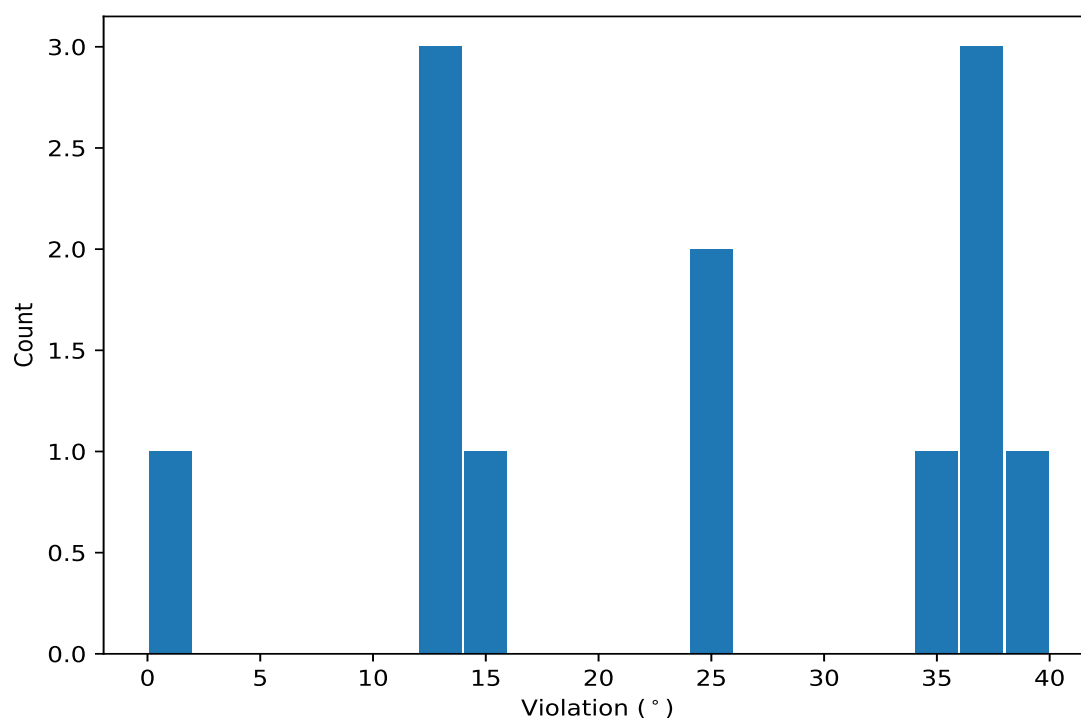
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,129)	1:28:A:G:C3'	1:28:A:G:O3'	1:29:A:A:P	1:29:A:A:O5'	9	26.77	11.71	35.38
(1,158)	1:37:A:A:C3'	1:37:A:A:O3'	1:38:A:U:P	1:38:A:U:O5'	2	24.96	0.06	24.96

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table provides the list of violations for 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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,129)	1:28:A:G:C3'	1:28:A:G:O3'	1:29:A:A:P	1:29:A:A:O5'	1	38.06
(1,129)	1:28:A:G:C3'	1:28:A:G:O3'	1:29:A:A:P	1:29:A:A:O5'	5	37.97
(1,129)	1:28:A:G:C3'	1:28:A:G:O3'	1:29:A:A:P	1:29:A:A:O5'	8	37.95
(1,129)	1:28:A:G:C3'	1:28:A:G:O3'	1:29:A:A:P	1:29:A:A:O5'	6	36.7
(1,129)	1:28:A:G:C3'	1:28:A:G:O3'	1:29:A:A:P	1:29:A:A:O5'	4	35.38
(1,158)	1:37:A:A:C3'	1:37:A:A:O3'	1:38:A:U:P	1:38:A:U:O5'	9	25.02
(1,158)	1:37:A:A:C3'	1:37:A:A:O3'	1:38:A:U:P	1:38:A:U:O5'	10	24.9
(1,129)	1:28:A:G:C3'	1:28:A:G:O3'	1:29:A:A:P	1:29:A:A:O5'	9	14.43
(1,129)	1:28:A:G:C3'	1:28:A:G:O3'	1:29:A:A:P	1:29:A:A:O5'	2	13.54
(1,129)	1:28:A:G:C3'	1:28:A:G:O3'	1:29:A:A:P	1:29:A:A:O5'	3	13.47