Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2MVY
BMRB ID	:	25291
Title	:	Structure and Stability of RNAs Containing N6-Methyl-adenosine
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Deposited on	:	2014-10-20

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

We welcome your comments at *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 (i) 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 (i)) were used in the production of this report:

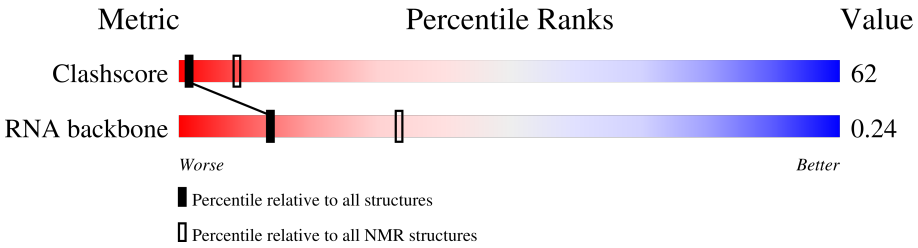
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 29%.

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	158937	12864
RNA backbone	4643	676

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 <=5%

Mol	Chain	Length	Quality of chain
1	1	10	100%
1	2	10	10% 90%

2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 640 atoms, of which 220 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called RNA.

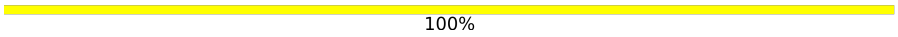
Mol	Chain	Residues	Atoms						Trace
1	1	10	Total	C	H	N	O	P	0
			320	95	110	38	68	9	
1	2	10	Total	C	H	N	O	P	0
			320	95	110	38	68	9	

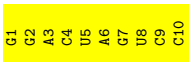
4 Residue-property plots (i)

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

Chain 1:





- Molecule 1: RNA

Chain 2:

5 Refinement protocol and experimental data overview

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

Of the 30 calculated structures, 1 were deposited, based on the following criterion: *target function.*

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

Software name	Classification	Version
X-PLOR NIH	structure solution	2.36
X-PLOR NIH	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	133
Number of shifts mapped to atoms	133
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	29%

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	1	210	110	110	24
1	2	210	110	110	16
All	All	420	220	220	40

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 62.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:1:5:U:O2'	1:1:6:A:H5'	1.00	1.54
1:2:13:A:H2'	1:2:14:C:C6	0.95	1.95
1:1:6:A:O2'	1:1:7:G:H5'	0.88	1.67
1:1:7:G:O2'	1:1:8:U:H5'	0.88	1.68
1:2:17:G:O2'	1:2:18:U:H5'	0.85	1.72
1:1:5:U:HO2'	1:1:6:A:H5'	0.73	1.40
1:2:16:A:O2'	1:2:17:G:H5'	0.73	1.82
1:1:5:U:O2'	1:1:6:A:C5'	0.72	2.33
1:2:11:G:O2'	1:2:12:G:H5'	0.71	1.85
1:1:1:G:O2'	1:1:2:G:H5'	0.70	1.87
1:2:13:A:C2	1:2:14:C:C2	0.68	2.81
1:2:12:G:H2'	1:2:13:A:C8	0.65	2.27
1:1:8:U:O2'	1:1:9:C:H5'	0.64	1.92
1:1:3:A:O2'	1:1:4:C:H5'	0.63	1.93

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:1:2:G:H2'	1:1:3:A:C8	0.61	2.31
1:2:11:G:H2'	1:2:12:G:C8	0.60	2.30
1:2:13:A:H2'	1:2:14:C:H6	0.60	1.51
1:1:7:G:O2'	1:1:8:U:C5'	0.58	2.47
1:1:1:G:H2'	1:1:2:G:C8	0.58	2.34
1:1:6:A:HO2'	1:1:7:G:H5'	0.56	1.61
1:1:5:U:H2'	1:1:6:A:C8	0.56	2.35
1:1:3:A:H2'	1:1:4:C:C6	0.55	2.36
1:1:9:C:H2'	1:1:10:C:C6	0.53	2.39
1:2:19:C:H2'	1:2:20:C:C6	0.52	2.40
1:1:4:C:H2'	1:1:5:U:C6	0.51	2.40
1:2:18:U:H2'	1:2:19:C:C6	0.51	2.40
1:2:17:G:H2'	1:2:18:U:C6	0.51	2.41
1:1:7:G:H2'	1:1:8:U:C6	0.50	2.42
1:1:6:A:O2'	1:1:7:G:C5'	0.49	2.52
1:1:6:A:H2'	1:1:7:G:C8	0.48	2.44
1:1:1:G:C6	1:1:2:G:C6	0.48	3.02
1:1:5:U:H2'	1:1:6:A:H8	0.48	1.68
1:1:7:G:HO2'	1:1:8:U:H5'	0.47	1.68
1:2:18:U:O2'	1:2:19:C:H5'	0.47	2.09
1:2:19:C:O2'	1:2:20:C:H5'	0.47	2.09
1:1:4:C:O2'	1:1:5:U:H5'	0.46	2.10
1:2:11:G:C6	1:2:12:G:C6	0.45	3.05
1:1:8:U:H2'	1:1:9:C:C6	0.44	2.48
1:2:17:G:HO2'	1:2:18:U:H5'	0.42	1.73
1:2:13:A:C2	1:2:14:C:O2	0.41	2.73

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	1	9/10 (90%)	0 (0%)	0 (0%)	0.28
1	2	9/10 (90%)	0 (0%)	0 (0%)	0.21
All	All	18/20 (90%)	0 (0%)	0 (0%)	0.24

The overall RNA backbone suiteness is 0.24.

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 monosaccharides 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 29% for the well-defined parts and 29% 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	133
Number of shifts mapped to atoms	133
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

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

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 29%, i.e. 111 atoms were assigned a chemical shift out of a possible 378. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Sugar	69/220 (31%)	38/120 (32%)	31/100 (31%)	0/0 (—%)
Base	42/158 (27%)	27/98 (28%)	15/34 (44%)	0/26 (0%)
Overall	111/378 (29%)	65/218 (30%)	46/134 (34%)	0/26 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 29%, i.e. 111 atoms were assigned a chemical shift out of a possible 378. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Sugar	69/220 (31%)	38/120 (32%)	31/100 (31%)	0/0 (—%)
Base	42/158 (27%)	27/98 (28%)	15/34 (44%)	0/26 (0%)
Overall	111/378 (29%)	65/218 (30%)	46/134 (34%)	0/26 (0%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

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	382
Intra-residue (|i-j|=0)	160
Sequential (|i-j|=1)	142
Medium range (|i-j|>1 and |i-j|<5)	0
Long range (|i-j|≥5)	0
Inter-chain	80
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	172
Number of unmapped restraints	0
Number of restraints per residue	27.7
Number of long range restraints per residue[1]	0.0

[1]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)	13.0	0.19
0.2-0.5 (Medium)	11.0	0.44
>0.5 (Large)	4.0	0.96

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 (i)

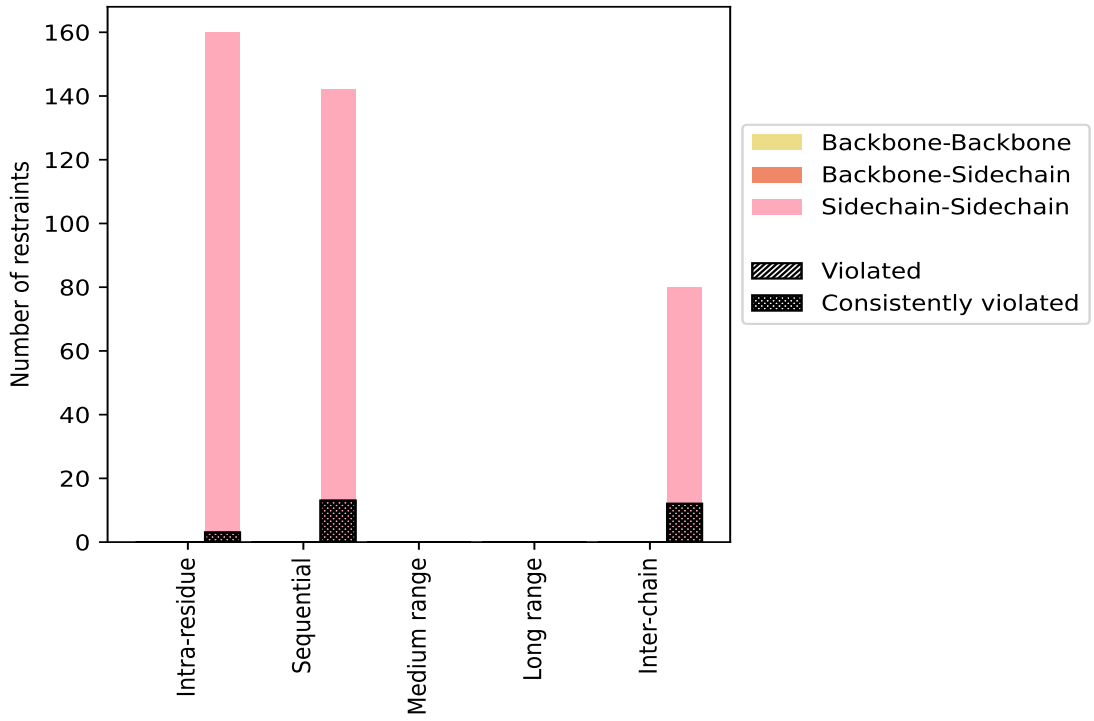
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	160	41.9	3	1.9	0.8	3	1.9	0.8
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	160	41.9	3	1.9	0.8	3	1.9	0.8
Sequential (|i-j|=1)	142	37.2	13	9.2	3.4	13	9.2	3.4
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	142	37.2	13	9.2	3.4	13	9.2	3.4
Medium range (|i-j|>1 & |i-j|<5)	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
Long range (|i-j|≥5)	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
Inter-chain	80	20.9	12	15.0	3.1	12	15.0	3.1
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	80	20.9	12	15.0	3.1	12	15.0	3.1
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	382	100.0	28	7.3	7.3	28	7.3	7.3
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	382	100.0	28	7.3	7.3	28	7.3	7.3

[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



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

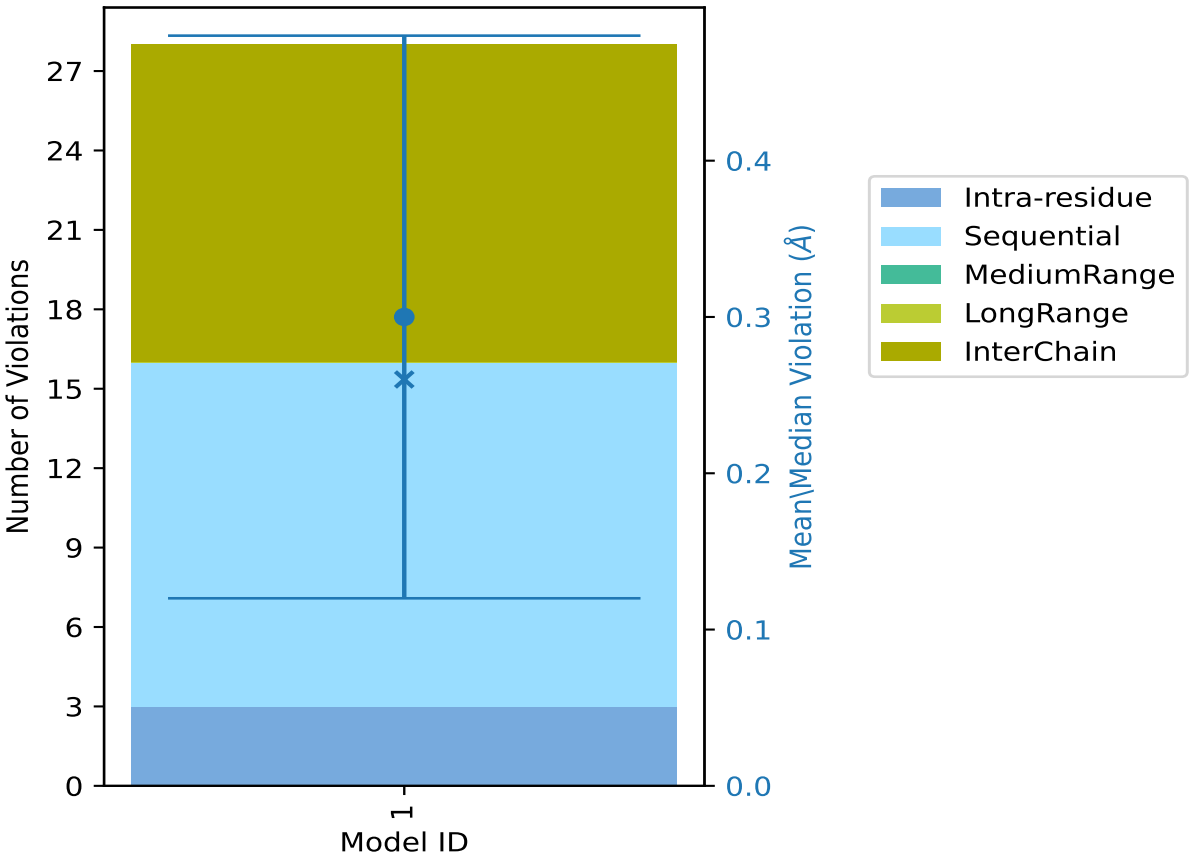
9.2 Distance violation statistics for each model

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	3	13	0	0	12	28	0.3	0.96	0.18	0.26

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

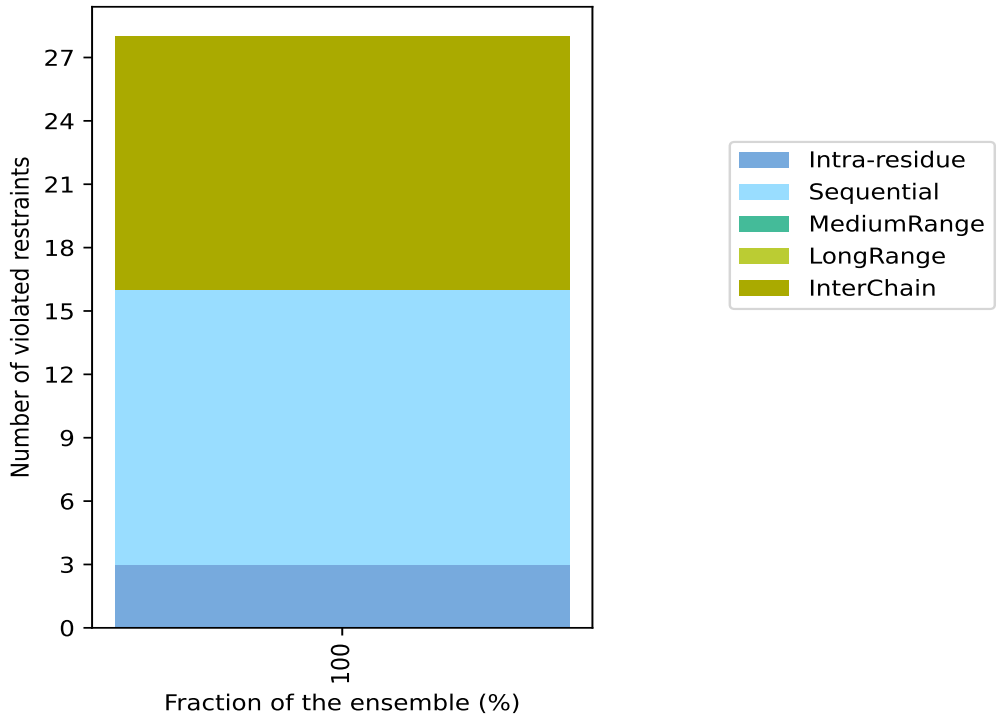
9.3 Distance violation statistics for the ensemble

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, 354(IR:157, SQ:129, MR:0, LR:0, IC:68) 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]	%
3	13	0	0	12	28	1	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

9.3.1 Bar graph : Distance violation statistics for the ensemble



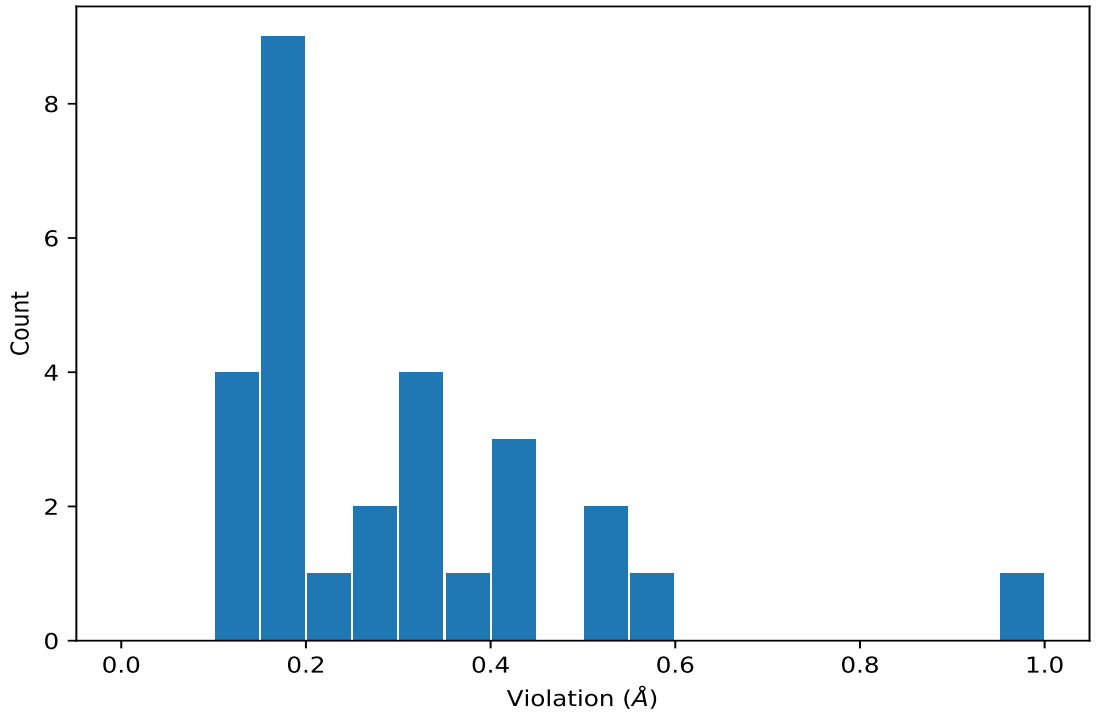
9.4 Most violated distance restraints in the ensemble

No violations found

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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 lists the absolute value of the violation for each restraint in the ensemble sorted by its 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)
(1,21)	1:1:6:A:H61	1:2:15:U:O4	1	0.96
(2,253)	1:2:14:C:H1'	1:2:15:U:H6	1	0.55
(2,265)	1:2:14:C:H3'	1:2:15:U:H5	1	0.51
(2,258)	1:2:14:C:H1'	1:2:15:U:H5'	1	0.51
(1,20)	1:1:6:A:N1	1:2:15:U:H3	1	0.44
(1,25)	1:1:7:G:O6	1:2:14:C:H41	1	0.42
(2,244)	1:2:13:A:H2'	1:2:14:C:H6	1	0.4
(1,28)	1:2:13:A:H61	1:1:8:U:O4	1	0.39
(1,23)	1:1:7:G:H21	1:2:14:C:O2	1	0.35
(1,15)	1:2:17:G:O6	1:1:4:C:H41	1	0.33
(1,11)	1:1:3:A:H61	1:2:18:U:O4	1	0.33
(2,120)	1:1:4:C:H2'	1:1:5:U:H5	1	0.32
(2,269)	1:2:14:C:H6	1:2:15:U:H6	1	0.3
(2,135)	1:1:5:U:H2'	1:1:6:A:H8	1	0.3
(2,171)	1:1:7:G:H8	1:1:8:U:H6	1	0.22
(2,75)	1:1:1:G:H2'	1:1:2:G:H8	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,287)	1:2:16:A:H1'	1:2:16:A:H5'	1	0.19
(2,215)	1:2:11:G:H2'	1:2:12:G:H8	1	0.19
(1,27)	1:2:13:A:N1	1:1:8:U:H3	1	0.19
(2,151)	1:1:6:A:H2'	1:1:7:G:H8	1	0.18
(2,111)	1:1:3:A:H8	1:1:4:C:H6	1	0.18
(1,9)	1:1:3:A:H2	1:2:18:U:O2	1	0.18
(2,311)	1:2:17:G:H8	1:2:18:U:H6	1	0.17
(1,2)	1:1:1:G:H21	1:2:20:C:O2	1	0.16
(2,2)	1:2:16:A:H2	1:1:5:U:H3	1	0.12
(2,101)	1:1:3:A:H2'	1:1:3:A:H2	1	0.12
(2,194)	1:1:9:C:H3'	1:1:9:C:H6	1	0.11
(1,35)	1:2:11:G:H21	1:1:10:C:N3	1	0.11

10 Dihedral-angle violation analysis

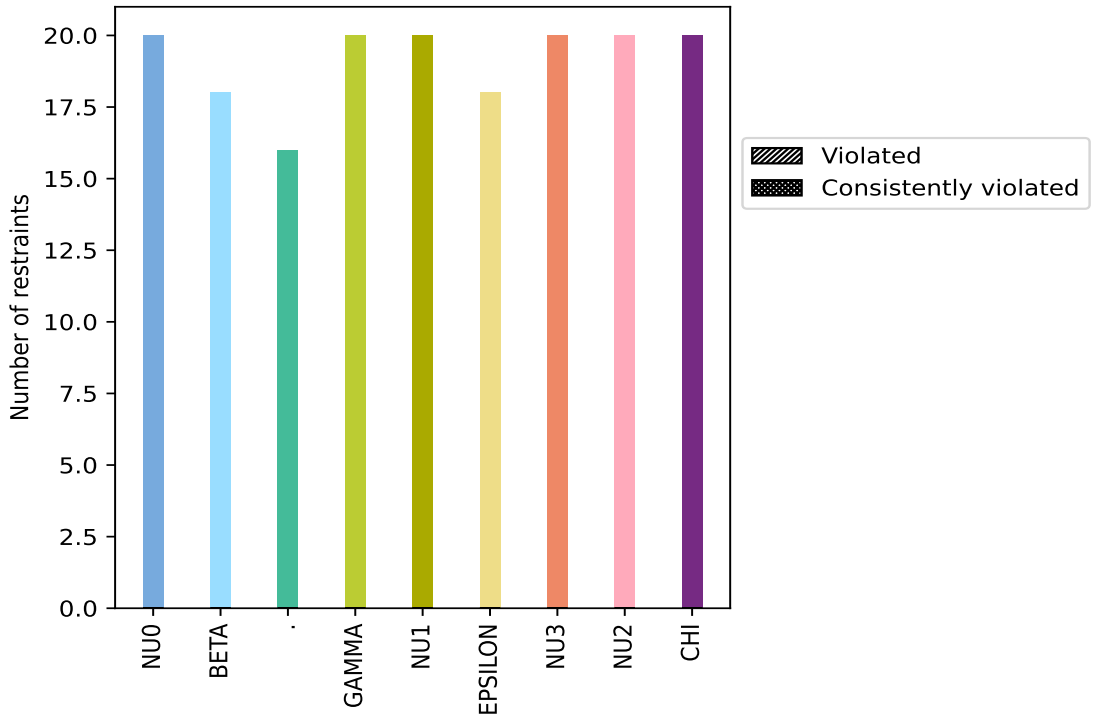
10.1 Summary of dihedral-angle violations

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]
NU0	20	11.6	0	0.0	0.0	0	0.0	0.0
BETA	18	10.5	0	0.0	0.0	0	0.0	0.0
.	16	9.3	0	0.0	0.0	0	0.0	0.0
GAMMA	20	11.6	0	0.0	0.0	0	0.0	0.0
NU1	20	11.6	0	0.0	0.0	0	0.0	0.0
EPSILON	18	10.5	0	0.0	0.0	0	0.0	0.0
NU3	20	11.6	0	0.0	0.0	0	0.0	0.0
NU2	20	11.6	0	0.0	0.0	0	0.0	0.0
CHI	20	11.6	0	0.0	0.0	0	0.0	0.0
Total	172	100.0	0	0.0	0.0	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



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

10.2 Dihedral-angle violation statistics for each model

No violations found

10.3 Dihedral-angle violation statistics for the ensemble

No violations found

10.4 Most violated dihedral-angle restraints in the ensemble

No violations found

10.5 All violated dihedral-angle restraints

No violations found