



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 9DKG / pdb_00009dkg
BMRB ID : 31201
Title : NMR structures of small molecules bound to a model of an RNA CAG repeat expansion.
Authors : Chen, J.L.; Taghavi, A.; Disney, M.D.; Fountain, M.A.; Childs-Disney, J.L.
Deposited on : 2024-09-08

This is a wwPDB NMR Structure Validation Summary 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 ⓘ 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

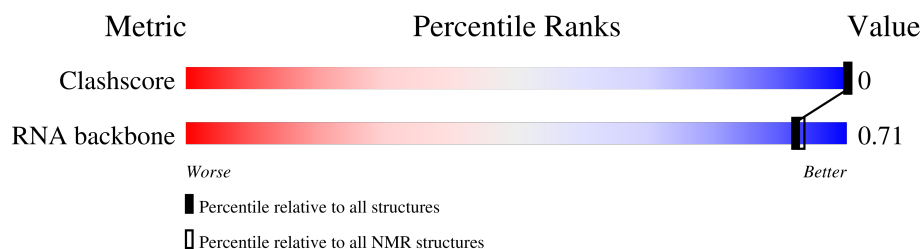
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

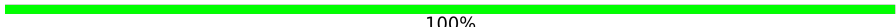
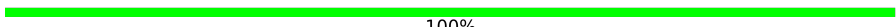
The overall completeness of chemical shifts assignment is 16%.

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	13	 100%
1	B	13	 100%

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 834 atoms, of which 284 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3').

Mol	Chain	Residues	Atoms						Trace
1	A	13	Total	C	H	N	O	P	0
			417	124	142	51	88	12	
1	B	13	Total	C	H	N	O	P	0
			417	124	142	51	88	12	

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: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

Chain B:  100%

There are no outlier residues in this chain.

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: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: CAG 13-mer RNA (5'-R(*GP*AP*CP*AP*GP*CP*AP*GP*CP*UP*GP*UP*C)-3')

Chain B:  100%

There are no outlier residues in this chain.

5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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
Amber	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	81
Number of shifts mapped to atoms	81
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	16%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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	B	0.0±0.0	0.5±0.6
1	A	0.0±0.0	0.4±0.7
All	All	0	18

There are no bond-length outliers.

There are no bond-angle outliers.

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	B	21	G	Sidechain	9
1	A	8	G	Sidechain	6
1	B	22	C	Sidechain	1
1	A	6	C	Sidechain	1
1	A	9	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
All	All	11000	5680	5720	-

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	12/13 (92%)	0±0 (0±0%)	0±0 (0±0%)	0.68±0.00
1	B	12/13 (92%)	0±0 (0±0%)	0±0 (0±0%)	0.69±0.00
All	All	480/520 (92%)	0 (0%)	0 (0%)	0.69

The overall RNA backbone suiteness is 0.71.

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 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 16% for the well-defined parts and 16% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *chem_shift_list_1*

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	81
Number of shifts mapped to atoms	81
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 [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 16%, i.e. 79 atoms were assigned a chemical shift out of a possible 494. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Sugar	46/286 (16%)	46/156 (29%)	0/130 (0%)	0/0 (—%)
Base	33/208 (16%)	33/130 (25%)	0/44 (0%)	0/34 (0%)
Overall	79/494 (16%)	79/286 (28%)	0/174 (0%)	0/34 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots

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 [i](#)

8.1 Conformationally restricting restraints [i](#)

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	285
Intra-residue ($ i-j =0$)	140
Sequential ($ i-j =1$)	84
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	29
Hydrogen bond restraints	32
Disulfide bond restraints	0
Total dihedral-angle restraints	140
Number of unmapped restraints	0
Number of restraints per residue	16.3
Number of long range restraints per residue ¹	0.0

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 [i](#)

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 [i](#)

Distance violations less than 0.1 Å are not included in the calculation. There are no distance violations

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)	None	None

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Bins (°)	Average number of violations per model	Max (°)
10.0-20.0 (Medium)	None	None
>20.0 (Large)	0.8	65.2

9 Distance violation analysis ⓘ

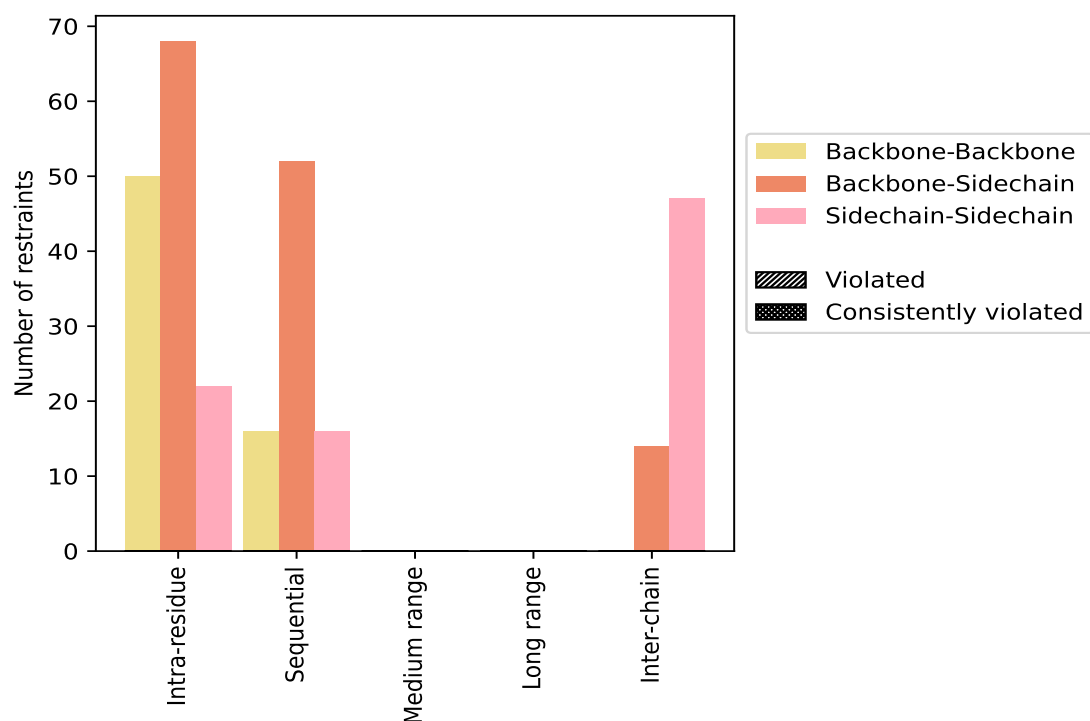
9.1 Summary of distance violations ⓘ

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)	140	49.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	50	17.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	68	23.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	22	7.7	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	84	29.5	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	16	5.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	52	18.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	16	5.6	0	0.0	0.0	0	0.0	0.0
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	29	10.2	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	14	4.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	15	5.3	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	32	11.2	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	285	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	66	23.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	134	47.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	85	29.8	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](#)

No violations found

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

No violations found

9.4 Most violated distance restraints in the ensemble [i](#)

No violations found

9.5 All violated distance restraints [i](#)

No violations found

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

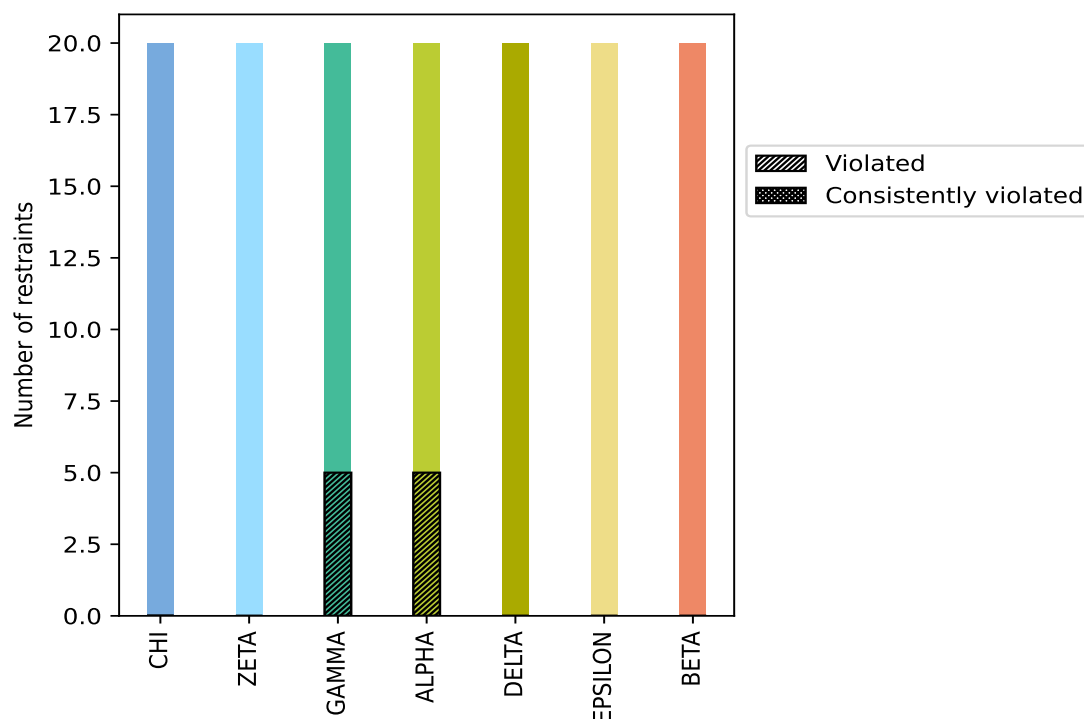
10.1 Summary of dihedral-angle violations [i](#)

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
CHI	20	14.3	0	0.0	0.0	0	0.0	0.0
ZETA	20	14.3	0	0.0	0.0	0	0.0	0.0
GAMMA	20	14.3	5	25.0	3.6	0	0.0	0.0
ALPHA	20	14.3	5	25.0	3.6	0	0.0	0.0
DELTA	20	14.3	0	0.0	0.0	0	0.0	0.0
EPSILON	20	14.3	0	0.0	0.0	0	0.0	0.0
BETA	20	14.3	0	0.0	0.0	0	0.0	0.0
Total	140	100.0	10	7.1	7.1	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](#)



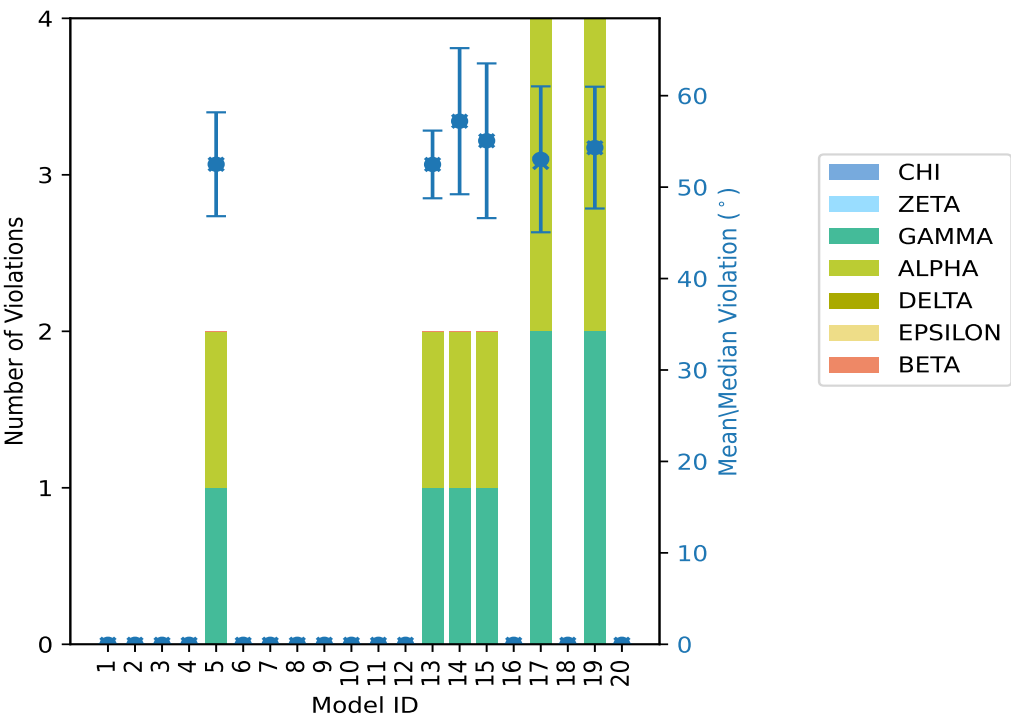
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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 (°)	SD (°)	Median (°)
	CHI	ZETA	GAMMA	ALPHA	DELTA	EPSILON	BETA	Total				
1	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	1	1	0	0	0	2	52.5	58.18	5.68	52.5
6	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	1	1	0	0	0	2	52.48	56.18	3.7	52.48
14	0	0	1	1	0	0	0	2	57.21	65.2	7.99	57.21
15	0	0	1	1	0	0	0	2	55.07	63.53	8.46	55.07
16	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
17	0	0	2	2	0	0	0	4	53.04	62.74	7.98	52.7
18	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	2	2	0	0	0	4	54.32	63.58	6.66	54.3
20	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0

10.2.1 Bar graph : Dihedral 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

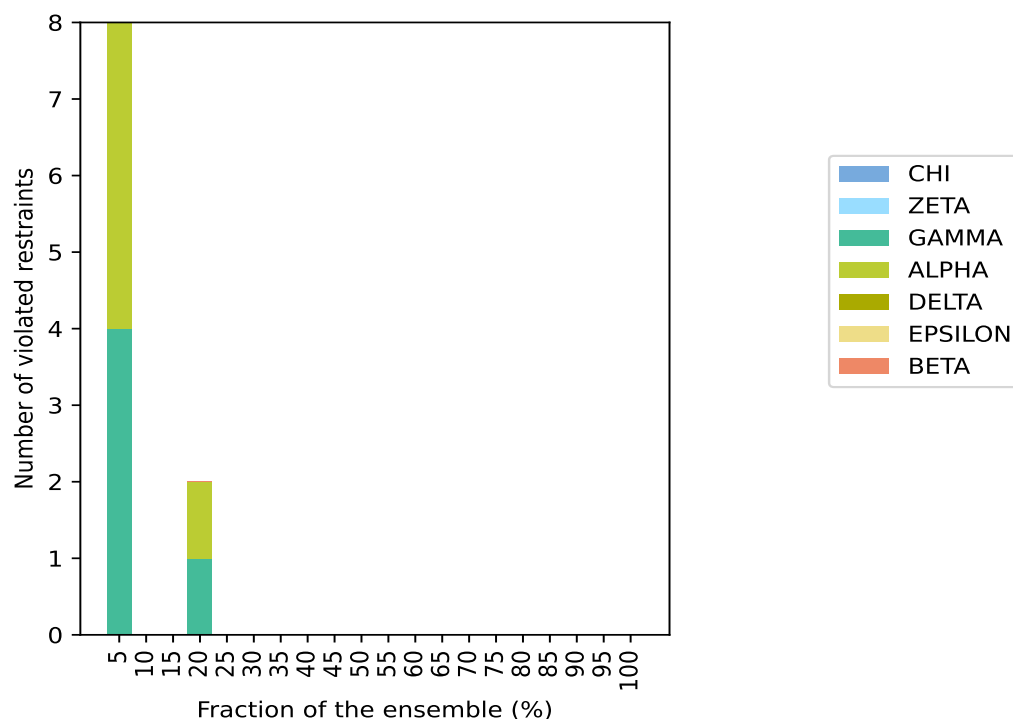
10.3 Dihedral-angle violation statistics for the ensemble

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	
CHI	ZETA	GAMMA	ALPHA	DELTA	EPSILON	BETA	Total	Count ¹	%
0	0	4	4	0	0	0	8	1	5.0
0	0	0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	0	0	3	15.0
0	0	1	1	0	0	0	2	4	20.0
0	0	0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	0	0	20	100.0

¹ Number of models with violations

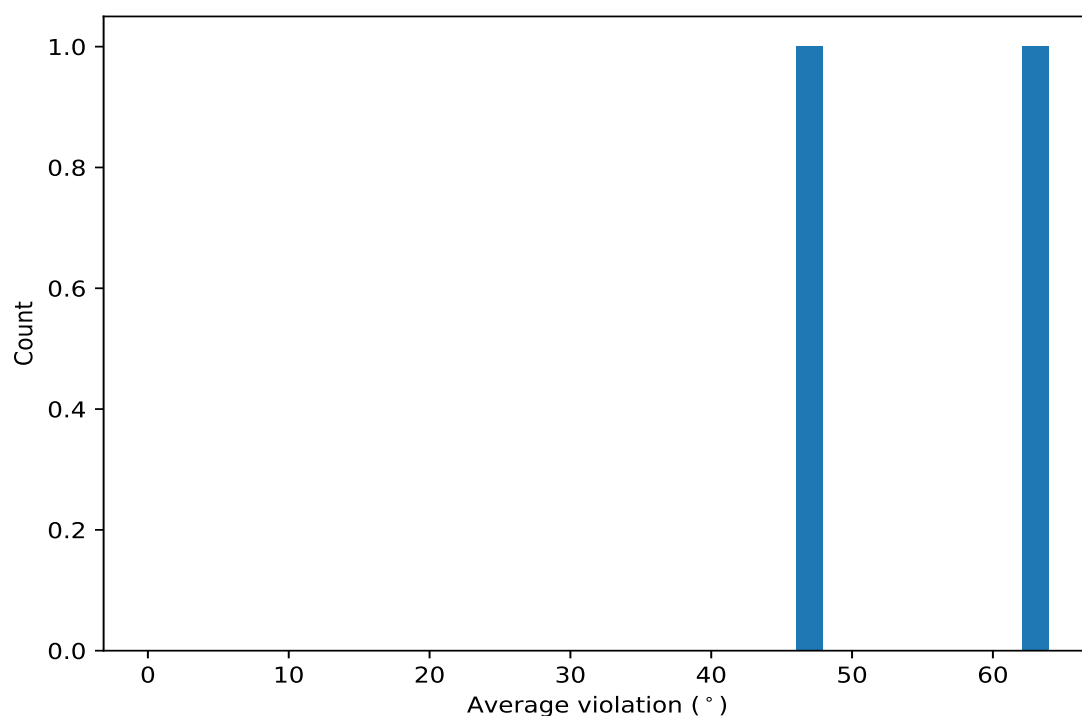
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

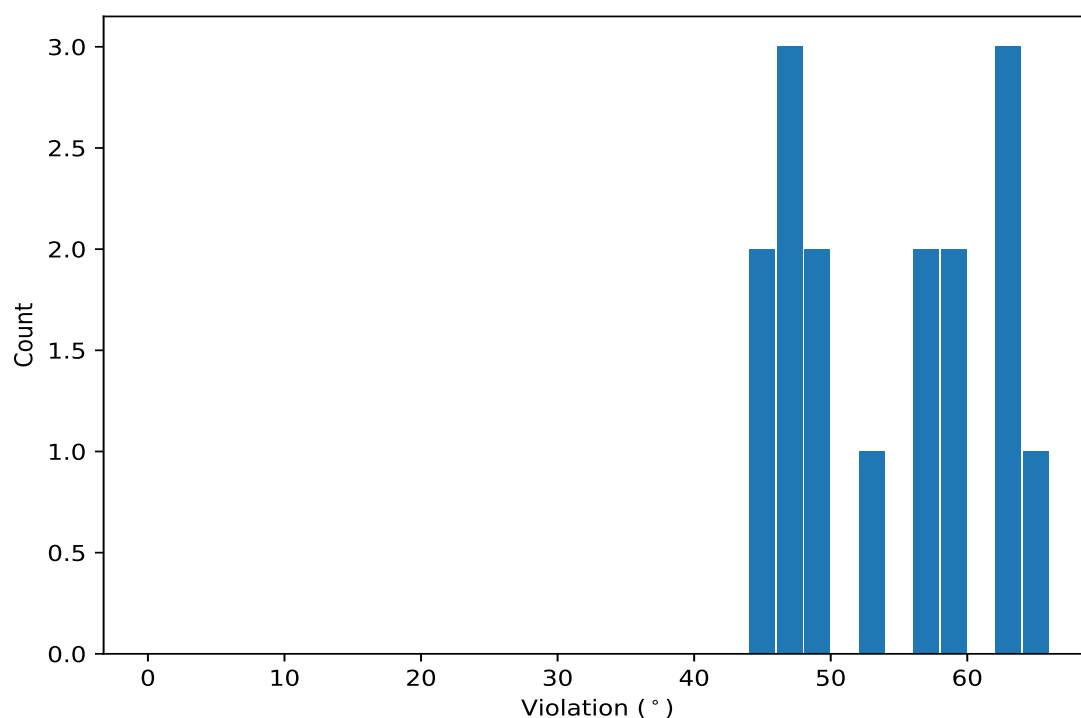
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,46)	1:8:A:G:O5'	1:8:A:G:C5'	1:8:A:G:C4'	1:8:A:G:C3'	4	63.76	0.89	63.56
(1,6)	1:7:A:A:O3'	1:8:A:G:P	1:8:A:G:O5'	1:8:A:G:C5'	4	46.84	1.49	46.51

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 (°)
(1,46)	1:8:A:G:O5'	1:8:A:G:C5'	1:8:A:G:C4'	1:8:A:G:C3'	14	65.2
(1,46)	1:8:A:G:O5'	1:8:A:G:C5'	1:8:A:G:C4'	1:8:A:G:C3'	19	63.58
(1,46)	1:8:A:G:O5'	1:8:A:G:C5'	1:8:A:G:C4'	1:8:A:G:C3'	15	63.53
(1,46)	1:8:A:G:O5'	1:8:A:G:C5'	1:8:A:G:C4'	1:8:A:G:C3'	17	62.74
(1,56)	1:21:B:G:O5'	1:21:B:G:C5'	1:21:B:G:C4'	1:21:B:G:C3'	17	58.99
(1,41)	1:2:A:A:O5'	1:2:A:A:C5'	1:2:A:A:C4'	1:2:A:A:C3'	5	58.18
(1,49)	1:11:A:G:O5'	1:11:A:G:C5'	1:11:A:G:C4'	1:11:A:G:C3'	19	56.18
(1,44)	1:5:A:G:O5'	1:5:A:G:C5'	1:5:A:G:C4'	1:5:A:G:C3'	13	56.18
(1,9)	1:10:A:U:O3'	1:11:A:G:P	1:11:A:G:O5'	1:11:A:G:C5'	19	52.42
(1,6)	1:7:A:A:O3'	1:8:A:G:P	1:8:A:G:O5'	1:8:A:G:C5'	14	49.22