



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 10:42 AM UTC

PDB ID : 7EUC / pdb_00007euc
BMRB ID : 36421
Title : Parallel G-quadruplex structure
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Deposited on : 2021-05-17

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 ⓘ 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 : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
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 43%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

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 are 4 unique types of molecules in this entry. The entry contains 719 atoms, of which 256 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA (5'-D(*TP*TP*GP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms						Trace
1	A	6	Total	C	H	N	O	P	0
			194	60	69	24	36	5	

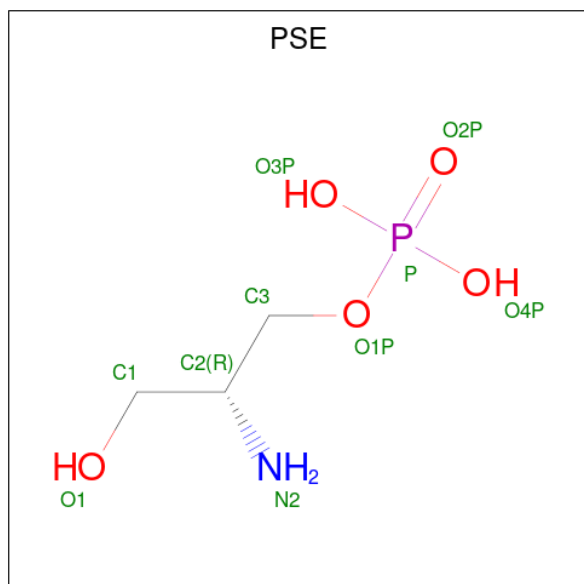
- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms						Trace
2	B	4	Total	C	H	N	O	P	0
			132	40	44	20	24	4	
2	C	4	Total	C	H	N	O	P	0
			132	40	44	20	24	4	

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*GP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms						Trace
3	D	5	Total	C	H	N	O	P	0
			165	50	57	22	31	5	

- Molecule 4 is O-PHOSPHOETHANOLAMINE (CCD ID: PSE) (formula: C₃H₁₀NO₅P).



Mol	Chain	Residues	Atoms					
4	A	1	Total	C	H	N	O	P
			16	3	7	1	4	1
4	B	1	Total	C	H	N	O	P
			16	3	7	1	4	1
4	B	1	Total	C	H	N	O	P
			16	3	7	1	4	1
4	C	1	Total	C	H	N	O	P
			16	3	7	1	4	1
4	C	1	Total	C	H	N	O	P
			16	3	7	1	4	1
4	D	1	Total	C	H	N	O	P
			16	3	7	1	4	1

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: DNA (5'-D(*TP*TP*GP*GP*GP*G)-3')

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 3: DNA (5'-D(P*GP*GP*GP*GP*T)-3')

Chain D:  100%

There are no outlier residues in this chain.

4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

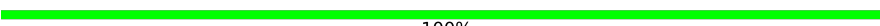
4.2.1 Score per residue for model 1

- Molecule 1: DNA (5'-D(*TP*TP*GP*GP*GP*G)-3')

Chain A:  100%

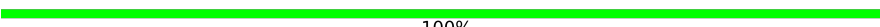
There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain B:  100%

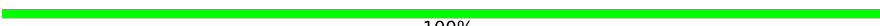
There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain C:  100%

There are no outlier residues in this chain.

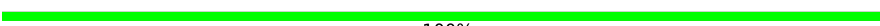
- Molecule 3: DNA (5'-D(P*GP*GP*GP*GP*T)-3')

Chain D:  100%

There are no outlier residues in this chain.

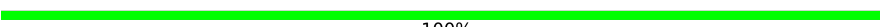
4.2.2 Score per residue for model 2

- Molecule 1: DNA (5'-D(*TP*TP*GP*GP*GP*G)-3')

Chain A:  100%

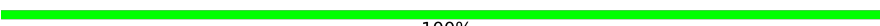
There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain B:  100%

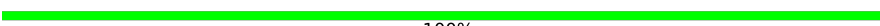
There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain C:  100%

There are no outlier residues in this chain.

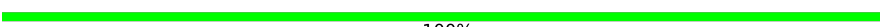
- Molecule 3: DNA (5'-D(P*GP*GP*GP*GP*T)-3')

Chain D:  100%

There are no outlier residues in this chain.

4.2.3 Score per residue for model 3

- Molecule 1: DNA (5'-D(*TP*TP*GP*GP*GP*G)-3')

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 3: DNA (5'-D(P*GP*GP*GP*GP*T)-3')

Chain D:  100%

There are no outlier residues in this chain.

4.2.4 Score per residue for model 4

- Molecule 1: DNA (5'-D(*TP*TP*GP*GP*GP*G)-3')

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 3: DNA (5'-D(P*GP*GP*GP*GP*T)-3')

Chain D:  100%

There are no outlier residues in this chain.

4.2.5 Score per residue for model 5

- Molecule 1: DNA (5'-D(*TP*TP*GP*GP*GP*G)-3')

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 3: DNA (5'-D(P*GP*GP*GP*GP*T)-3')

Chain D:  100%

There are no outlier residues in this chain.

4.2.6 Score per residue for model 6

- Molecule 1: DNA (5'-D(*TP*TP*GP*GP*GP*G)-3')

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 3: DNA (5'-D(P*GP*GP*GP*GP*T)-3')

Chain D:  100%

There are no outlier residues in this chain.

4.2.7 Score per residue for model 7

- Molecule 1: DNA (5'-D(*TP*TP*GP*GP*GP*G)-3')

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 3: DNA (5'-D(P*GP*GP*GP*GP*T)-3')

Chain D:  100%

There are no outlier residues in this chain.

4.2.8 Score per residue for model 8

- Molecule 1: DNA (5'-D(*TP*TP*GP*GP*GP*G)-3')

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 3: DNA (5'-D(P*GP*GP*GP*GP*T)-3')

Chain D:  100%

There are no outlier residues in this chain.

4.2.9 Score per residue for model 9

- Molecule 1: DNA (5'-D(*TP*TP*GP*GP*GP*G)-3')

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 3: DNA (5'-D(P*GP*GP*GP*GP*T)-3')

Chain D:  100%

There are no outlier residues in this chain.

4.2.10 Score per residue for model 10

- Molecule 1: DNA (5'-D(*TP*TP*GP*GP*GP*G)-3')

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain B:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(P*GP*GP*GP*G)-3')

Chain C:  100%

There are no outlier residues in this chain.

- Molecule 3: DNA (5'-D(P*GP*GP*GP*GP*T)-3')

Chain D:  100%

There are no outlier residues in this chain.

5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure calculation	
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	177
Number of shifts mapped to atoms	177
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	43%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 43% for the well-defined parts and 43% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	177
Number of shifts mapped to atoms	177
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 43%, i.e. 168 atoms were assigned a chemical shift out of a possible 390. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Sugar	133/228 (58%)	133/133 (100%)	0/95 (0%)	0/0 (—%)
Base	35/162 (22%)	35/105 (33%)	0/22 (0%)	0/35 (0%)
Overall	168/390 (43%)	168/238 (71%)	0/117 (0%)	0/35 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 43%, i.e. 168 atoms were assigned a chemical shift out of a possible 390. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Sugar	133/228 (58%)	133/133 (100%)	0/95 (0%)	0/0 (—%)
Base	35/162 (22%)	35/105 (33%)	0/22 (0%)	0/35 (0%)
Overall	168/390 (43%)	168/238 (71%)	0/117 (0%)	0/35 (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	422
Intra-residue ($ i-j =0$)	268
Sequential ($ i-j =1$)	55
Medium range ($ i-j >1$ and $ i-j <5$)	3
Long range ($ i-j \geq 5$)	0
Inter-chain	32
Hydrogen bond restraints	64
Disulfide bond restraints	0
Total dihedral-angle restraints	16
Number of unmapped restraints	0
Number of restraints per residue	17.5
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

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)	9.6	0.2
0.2-0.5 (Medium)	3.2	0.37
>0.5 (Large)	None	None

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

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

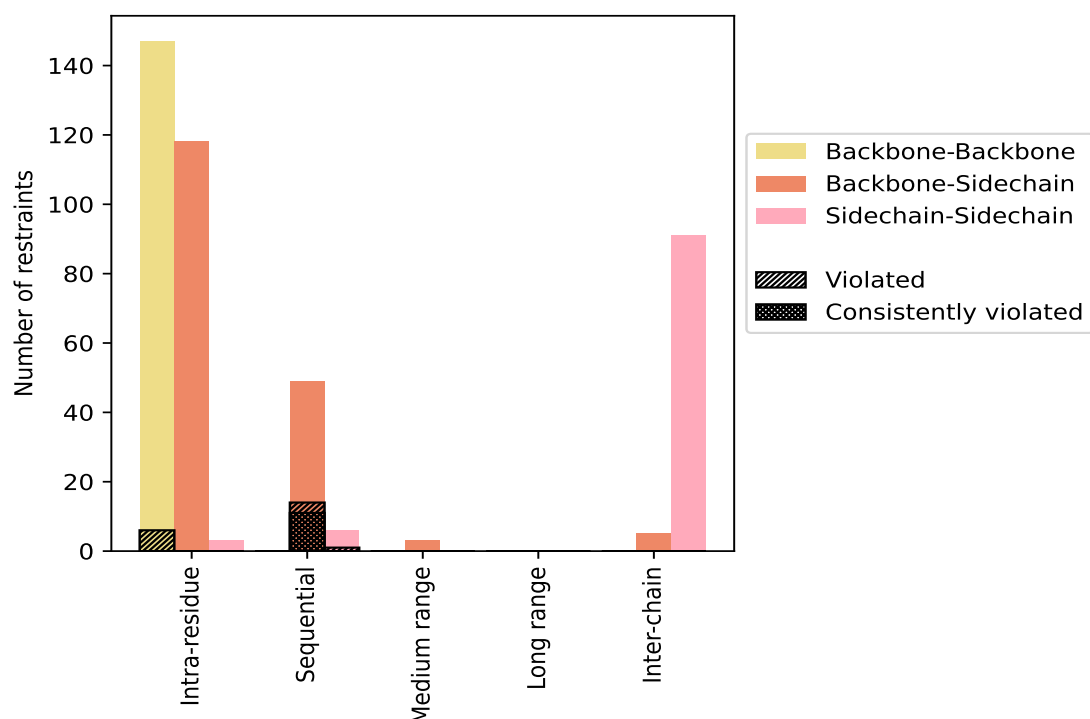
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($ i-j =0$)	268	63.5	6	2.2	1.4	0	0.0	0.0
Backbone-Backbone	147	34.8	6	4.1	1.4	0	0.0	0.0
Backbone-Sidechain	118	28.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	3	0.7	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	55	13.0	15	27.3	3.6	11	20.0	2.6
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	49	11.6	14	28.6	3.3	11	22.4	2.6
Sidechain-Sidechain	6	1.4	1	16.7	0.2	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	3	0.7	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	3	0.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range ($ i-j \geq 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	32	7.6	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	5	1.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	27	6.4	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	64	15.2	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	422	100.0	21	5.0	5.0	11	2.6	2.6
Backbone-Backbone	147	34.8	6	4.1	1.4	0	0.0	0.0
Backbone-Sidechain	175	41.5	14	8.0	3.3	11	6.3	2.6
Sidechain-Sidechain	100	23.7	1	1.0	0.2	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

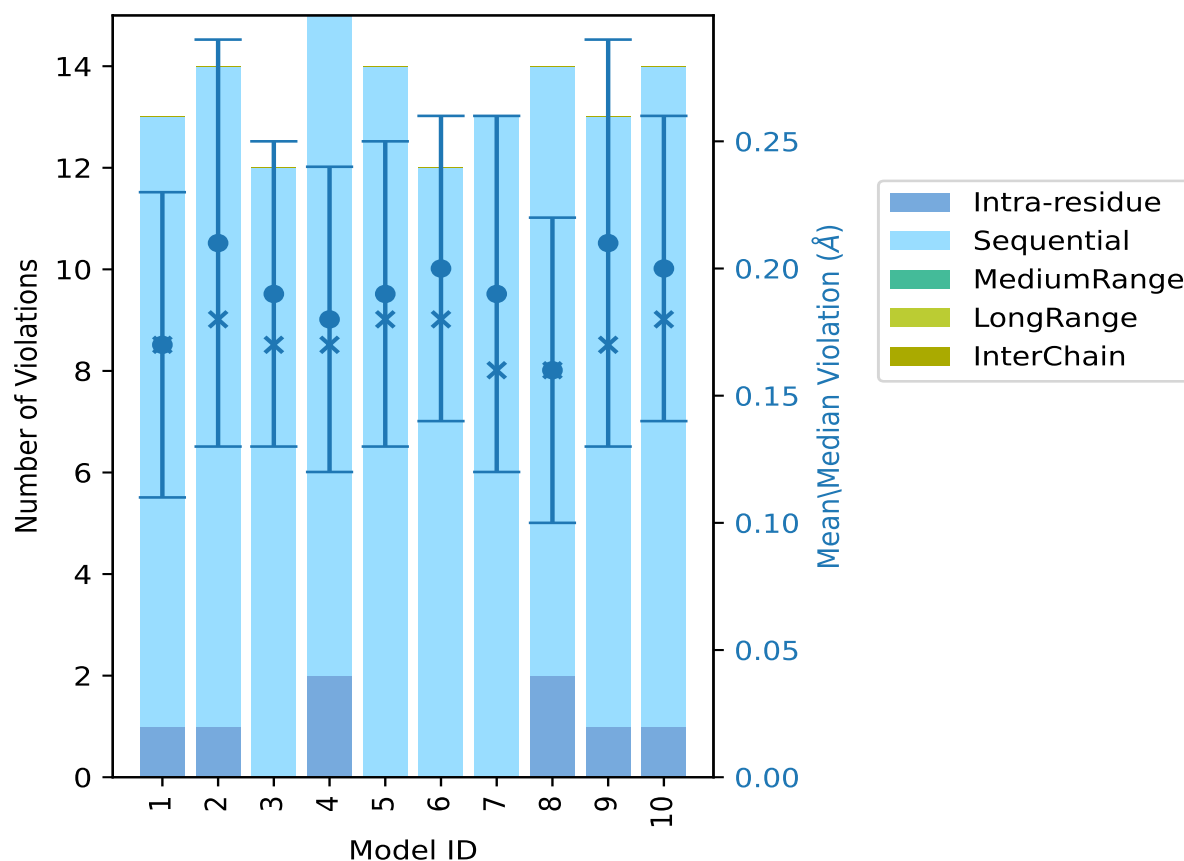
9.2 Distance violation statistics for each model [i](#)

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	1	12	0	0	0	13	0.17	0.35	0.06	0.17
2	1	13	0	0	0	14	0.21	0.37	0.08	0.18
3	0	12	0	0	0	12	0.19	0.36	0.06	0.17
4	2	13	0	0	0	15	0.18	0.36	0.06	0.17
5	0	14	0	0	0	14	0.19	0.35	0.06	0.18
6	0	12	0	0	0	12	0.2	0.36	0.06	0.18
7	0	13	0	0	0	13	0.19	0.35	0.07	0.16
8	2	12	0	0	0	14	0.16	0.36	0.06	0.16
9	1	12	0	0	0	13	0.21	0.36	0.08	0.17
10	1	13	0	0	0	14	0.2	0.37	0.06	0.18

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, 337(IR:262, SQ:40, MR:3, LR:0, IC:32) 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	%
4	1	0	0	0	5	1	10.0
2	0	0	0	0	2	2	20.0
0	2	0	0	0	2	3	30.0

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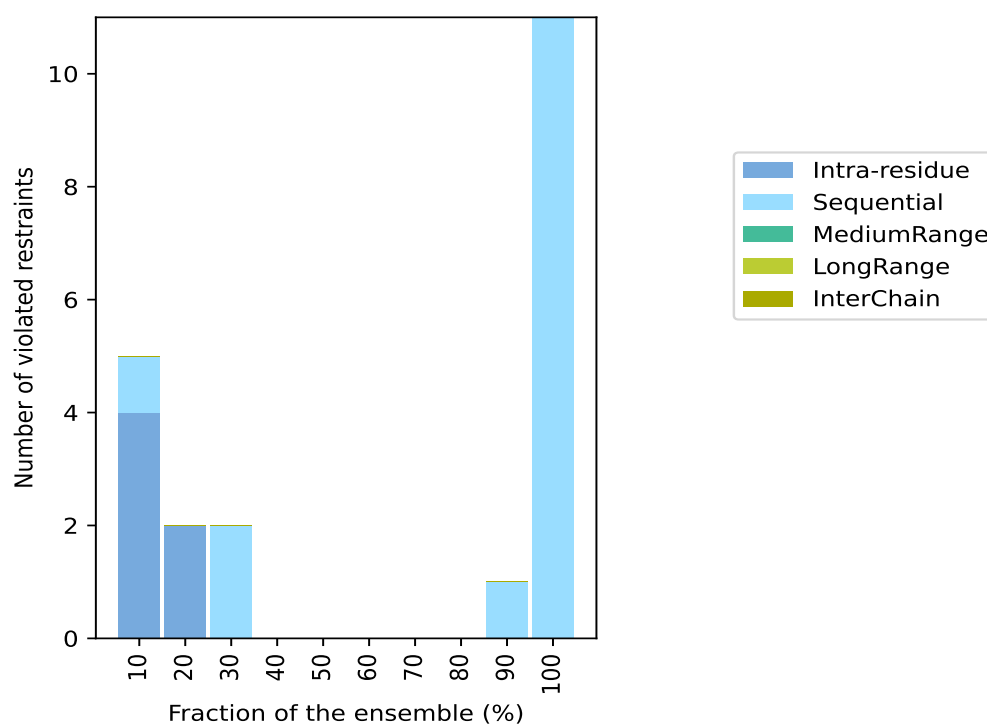
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	4	40.0
0	0	0	0	0	0	5	50.0
0	0	0	0	0	0	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	0	0	0	8	80.0
0	1	0	0	0	1	9	90.0
0	11	0	0	0	11	10	100.0

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 [i](#)

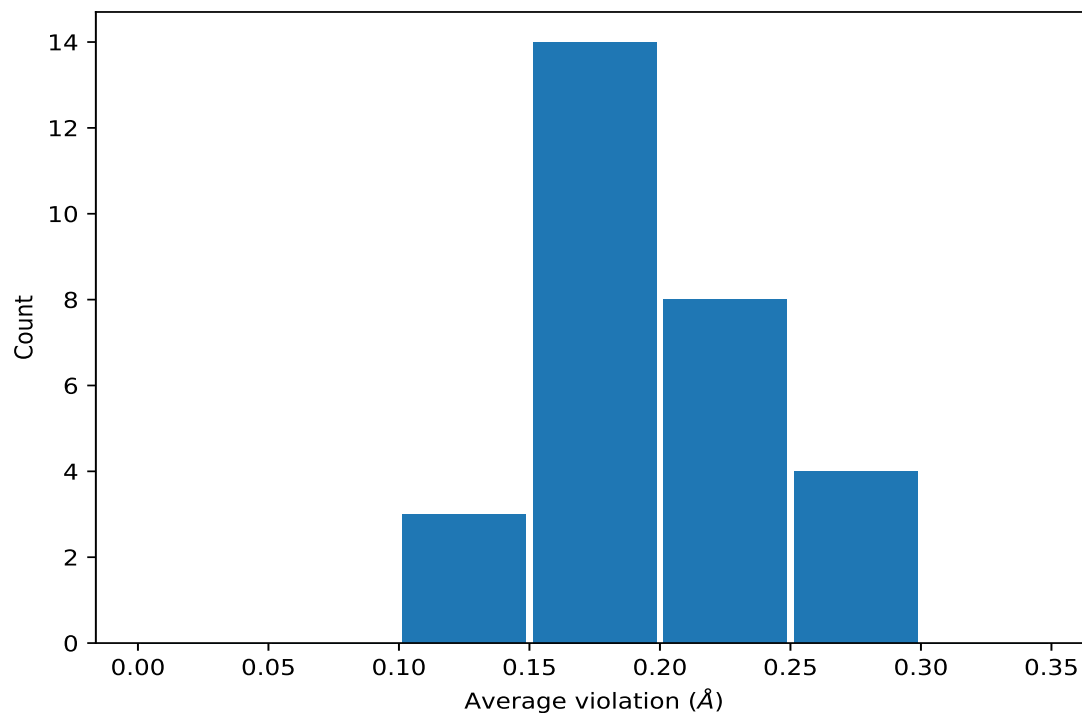


9.4 Most violated distance restraints in the ensemble [i](#)

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 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. 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)
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2'	10	0.27	0.09	0.29
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2''	10	0.27	0.09	0.29
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2'	10	0.21	0.08	0.18
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2''	10	0.21	0.08	0.18
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2'	10	0.2	0.05	0.18
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2''	10	0.2	0.05	0.18
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2'	10	0.2	0.09	0.18
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2''	10	0.2	0.09	0.18
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2'	10	0.19	0.03	0.18
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2''	10	0.19	0.03	0.18
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2'	10	0.19	0.06	0.17
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2''	10	0.19	0.06	0.17
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2'	10	0.18	0.01	0.18
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2''	10	0.18	0.01	0.18
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2'	10	0.18	0.01	0.18

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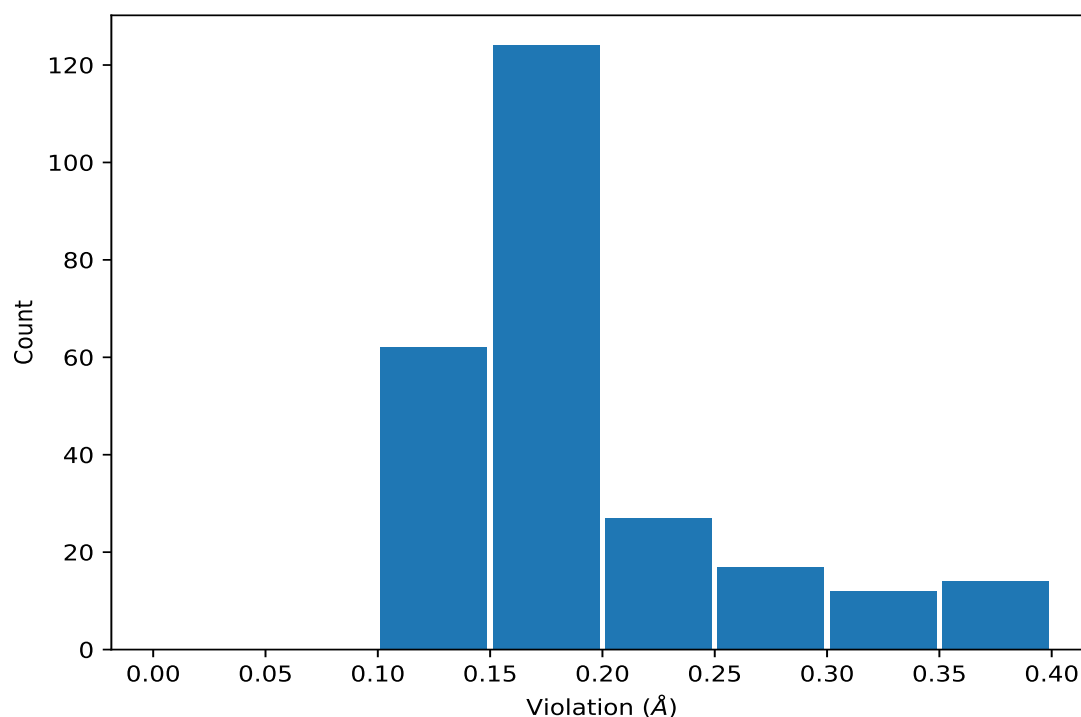
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2''	10	0.18	0.01	0.18
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2'	10	0.17	0.02	0.17
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2''	10	0.17	0.02	0.17
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2'	10	0.17	0.02	0.17
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2''	10	0.17	0.02	0.17
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2'	10	0.16	0.02	0.16
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2''	10	0.16	0.02	0.16
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2'	9	0.22	0.11	0.15
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2''	9	0.22	0.11	0.15
(1,166)	3:25:D:DT:H6	3:24:D:DG:H2'	3	0.26	0.02	0.27
(1,166)	3:25:D:DT:H6	3:24:D:DG:H2''	3	0.26	0.02	0.27
(2,4)	1:3:A:DG:H1	1:2:A:DT:C7	3	0.12	0.01	0.12
(1,281)	3:25:D:DT:H3'	3:25:D:DT:H5''	2	0.14	0.01	0.14
(1,205)	3:21:D:DG:H1'	3:21:D:DG:H4'	2	0.1	0.0	0.1

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

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)
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2'	10	0.37
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2''	10	0.37
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2'	2	0.37
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2''	2	0.37
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2'	4	0.36
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2''	4	0.36
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2'	8	0.36
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2''	8	0.36
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2'	3	0.36
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2''	3	0.36
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2'	6	0.36
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2''	6	0.36
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2'	9	0.36
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2''	9	0.36
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2'	5	0.35
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2''	5	0.35
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2'	7	0.35
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2''	7	0.35
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2'	1	0.35
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2''	1	0.35
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2'	2	0.35
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2''	2	0.35
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2'	9	0.34
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2''	9	0.34
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2'	7	0.33
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2''	7	0.33
(1,280)	3:25:D:DT:H3'	3:25:D:DT:H5'	9	0.3
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2'	2	0.3
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2''	2	0.3
(1,166)	3:25:D:DT:H6	3:24:D:DG:H2'	2	0.28
(1,166)	3:25:D:DT:H6	3:24:D:DG:H2''	2	0.28
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2'	9	0.28
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2''	9	0.28
(1,166)	3:25:D:DT:H6	3:24:D:DG:H2'	5	0.27
(1,166)	3:25:D:DT:H6	3:24:D:DG:H2''	5	0.27
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2'	4	0.27
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2''	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2'	6	0.27
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2''	6	0.27
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2'	3	0.26
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2''	3	0.26
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2'	10	0.25
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2''	10	0.25
(1,166)	3:25:D:DT:H6	3:24:D:DG:H2'	10	0.24
(1,166)	3:25:D:DT:H6	3:24:D:DG:H2''	10	0.24
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2'	9	0.24
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2''	9	0.24
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2'	6	0.23
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2''	6	0.23
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2'	8	0.23
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2''	8	0.23
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2'	7	0.22
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2''	7	0.22
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2'	6	0.22
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2''	6	0.22
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2'	10	0.22
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2''	10	0.22
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2'	2	0.22
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2''	2	0.22
(1,193)	1:3:A:DG:H1'	1:3:A:DG:H4'	10	0.21
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2'	5	0.21
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2''	5	0.21
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2'	1	0.2
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2''	1	0.2
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2'	10	0.2
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2''	10	0.2
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2'	4	0.2
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2''	4	0.2
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2'	7	0.2
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2''	7	0.2
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2'	3	0.19
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2''	3	0.19
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2'	5	0.19
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2''	5	0.19
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2'	2	0.19
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2''	2	0.19
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2'	7	0.19
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2''	7	0.19
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2'	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2''	4	0.19
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2'	2	0.19
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2''	2	0.19
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2'	5	0.19
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2''	5	0.19
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2'	10	0.19
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2''	10	0.19
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2'	8	0.19
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2''	8	0.19
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2'	1	0.18
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2''	1	0.18
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2'	2	0.18
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2''	2	0.18
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2'	10	0.18
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2''	10	0.18
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2'	3	0.18
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2''	3	0.18
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2'	6	0.18
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2''	6	0.18
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2'	1	0.18
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2''	1	0.18
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2'	4	0.18
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2''	4	0.18
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2'	5	0.18
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2''	5	0.18
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2'	6	0.18
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2''	6	0.18
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2'	8	0.18
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2''	8	0.18
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2'	10	0.18
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2''	10	0.18
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2'	5	0.18
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2''	5	0.18
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2'	6	0.18
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2''	6	0.18
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2'	2	0.18
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2''	2	0.18
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2'	3	0.18
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2''	3	0.18
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2'	5	0.18
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2''	5	0.18
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2'	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2''	9	0.18
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2'	4	0.18
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2''	4	0.18
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2'	10	0.18
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2''	10	0.18
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2'	4	0.18
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2''	4	0.18
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2'	5	0.18
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2''	5	0.18
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2'	4	0.17
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2''	4	0.17
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2'	1	0.17
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2''	1	0.17
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2'	10	0.17
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2''	10	0.17
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2'	3	0.17
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2''	3	0.17
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2'	9	0.17
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2''	9	0.17
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2'	1	0.17
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2''	1	0.17
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2'	4	0.17
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2''	4	0.17
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2'	8	0.17
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2''	8	0.17
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2'	10	0.17
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2''	10	0.17
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2'	1	0.17
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2''	1	0.17
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2'	6	0.17
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2''	6	0.17
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2'	7	0.17
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2''	7	0.17
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2'	1	0.17
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2''	1	0.17
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2'	6	0.17
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2''	6	0.17
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2'	9	0.17
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2''	9	0.17
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2'	9	0.17
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2''	9	0.17
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2'	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2''	1	0.17
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2'	3	0.17
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2''	3	0.17
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2'	6	0.17
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2''	6	0.17
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2'	3	0.17
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2''	3	0.17
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2'	5	0.17
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2''	5	0.17
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2'	10	0.17
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2''	10	0.17
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2'	8	0.16
(1,163)	3:24:D:DG:H8	3:23:D:DG:H2''	8	0.16
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2'	5	0.16
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2''	5	0.16
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2'	9	0.16
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2''	9	0.16
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2'	3	0.16
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2''	3	0.16
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2'	7	0.16
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2''	7	0.16
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2'	9	0.16
(1,149)	2:17:C:DG:H8	2:16:C:DG:H2''	9	0.16
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2'	8	0.16
(1,141)	2:12:B:DG:H8	2:11:B:DG:H2''	8	0.16
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2'	7	0.16
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2''	7	0.16
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2'	4	0.16
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2''	4	0.16
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2'	7	0.16
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2''	7	0.16
(1,281)	3:25:D:DT:H3'	3:25:D:DT:H5''	4	0.15
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2'	4	0.15
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2''	4	0.15
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2'	7	0.15
(1,160)	3:23:D:DG:H8	3:22:D:DG:H2''	7	0.15
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2'	2	0.15
(1,152)	2:18:C:DG:H8	2:17:C:DG:H2''	2	0.15
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2'	3	0.15
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2''	3	0.15
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2'	3	0.15
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2''	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2'	2	0.15
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2''	2	0.15
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2'	8	0.15
(1,130)	1:6:A:DG:H8	1:5:A:DG:H2''	8	0.15
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2'	1	0.15
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2''	1	0.15
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2'	3	0.15
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2''	3	0.15
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2'	4	0.15
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2''	4	0.15
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2'	8	0.14
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2''	8	0.14
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2'	9	0.14
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2''	9	0.14
(2,4)	1:3:A:DG:H1	1:2:A:DT:C7	7	0.13
(1,281)	3:25:D:DT:H3'	3:25:D:DT:H5''	8	0.13
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2'	5	0.13
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2''	5	0.13
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2'	7	0.13
(1,135)	2:10:B:DG:H8	2:9:B:DG:H2''	7	0.13
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2'	2	0.13
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2''	2	0.13
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2'	6	0.13
(1,127)	1:5:A:DG:H8	1:4:A:DG:H2''	6	0.13
(2,4)	1:3:A:DG:H1	1:2:A:DT:C7	5	0.12
(1,207)	3:23:D:DG:H1'	3:23:D:DG:H4'	8	0.12
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2'	1	0.12
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2''	1	0.12
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2'	2	0.12
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2''	2	0.12
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2'	7	0.12
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2''	7	0.12
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2'	6	0.11
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2''	6	0.11
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2'	9	0.11
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2''	9	0.11
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2'	10	0.11
(1,146)	2:16:C:DG:H8	2:15:C:DG:H2''	10	0.11
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2'	8	0.11
(1,138)	2:11:B:DG:H8	2:10:B:DG:H2''	8	0.11
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2'	1	0.11
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2''	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2'	5	0.11
(1,124)	1:4:A:DG:H8	1:3:A:DG:H2''	5	0.11
(2,4)	1:3:A:DG:H1	1:2:A:DT:C7	8	0.1
(1,205)	3:21:D:DG:H1'	3:21:D:DG:H4'	2	0.1
(1,205)	3:21:D:DG:H1'	3:21:D:DG:H4'	4	0.1
(1,197)	2:9:B:DG:H1'	2:9:B:DG:H4'	1	0.1
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2'	8	0.1
(1,157)	3:22:D:DG:H8	3:21:D:DG:H2''	8	0.1
(1,4)	1:3:A:DG:H8	1:2:A:DT:H1'	4	0.1

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

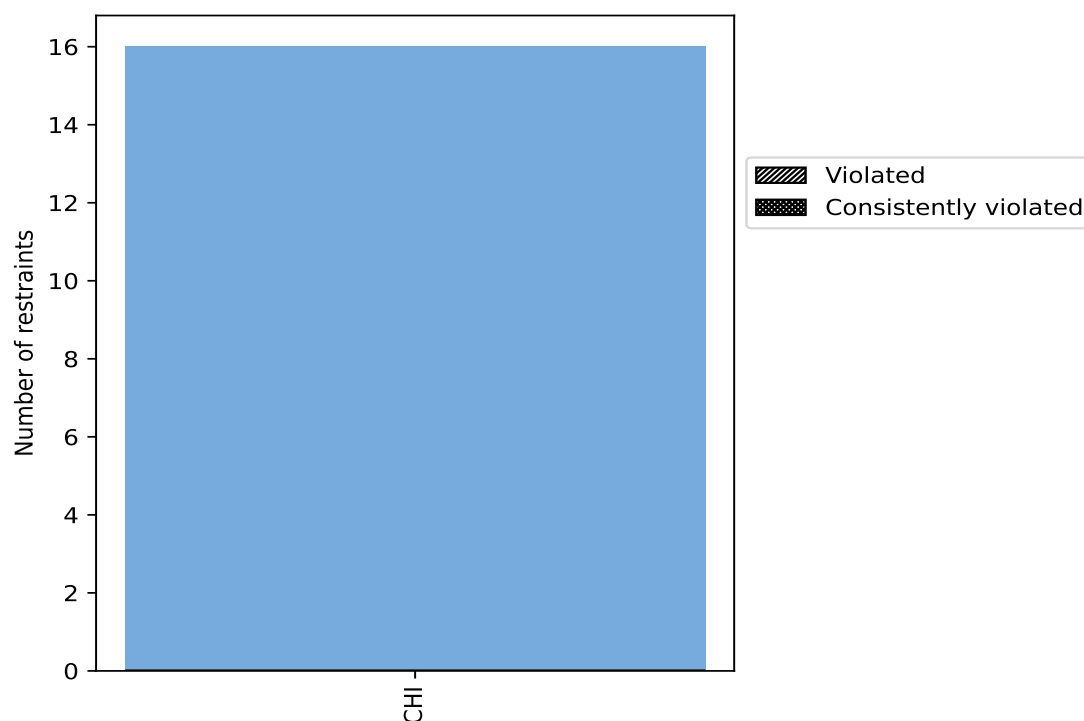
10.1 Summary of dihedral-angle violations [i](#)

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	16	100.0	0	0.0	0.0	0	0.0	0.0
Total	16	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 [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](#)

No violations found

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

No violations found

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

No violations found

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

No violations found