



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 24, 2025 – 02:21 PM JST

PDB ID : 9IO0  
BMRB ID : 36681  
Title : INTERACTION BETWEEN A FLUOROQUINOLONE DERIVATIVE  
KG022 AND RNAS: EFFECT OF BASE PAIRS 5' ADJACENT TO THE  
BULGE OUT ESIDUES  
Authors : Ichijo, R.; Kawai, G.  
Deposited on : 2024-07-08

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.41.4

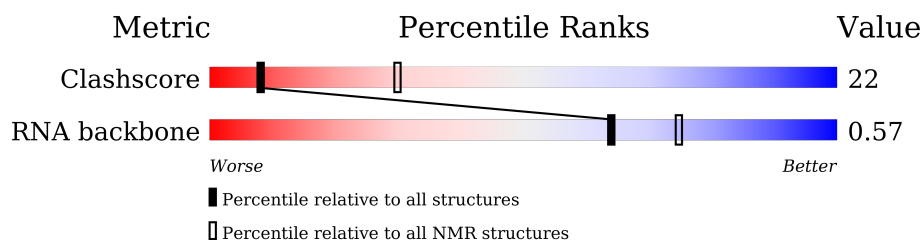
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

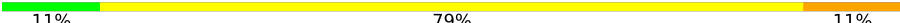
The overall completeness of chemical shifts assignment is 20%.

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	210492	14027
RNA backbone	6643	756

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	19	 <div> <span>11%</span> <span>79%</span> <span>11%</span> </div>

## 2 Ensemble composition and analysis ⓘ

This entry contains 11 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.

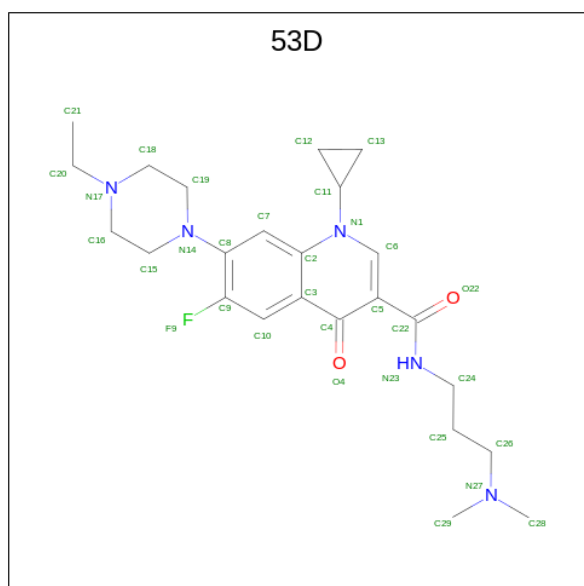
### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 673 atoms, of which 240 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	A	19	607	180	206	70	133	18	0

- Molecule 2 is 1-cyclopropyl-N-[3-(dimethylamino)propyl]-7-(4-ethylpiperazin-1-yl)-6-fluoranyl-4-oxidanylidene-quinoline-3-carboxamide (three-letter code: 53D) (formula: C<sub>24</sub>H<sub>34</sub>FN<sub>5</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					
			Total	C	F	H	N	O
2	A	1	66	24	1	34	5	2

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

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

Chain A: 




### 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: RNA (5'-R(\*GP\*GP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*CP\*GP\*AP\*CP\*CP\*GP\*AP\*UP\*CP\*C)-3')

Chain A: 



#### 4.2.2 Score per residue for model 2

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

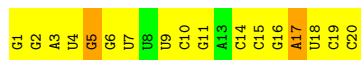
Chain A: 



### 4.2.3 Score per residue for model 3

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

Chain A:  11% 79% 11%



### 4.2.4 Score per residue for model 4

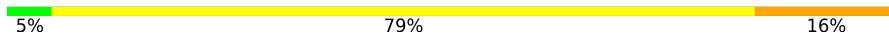
- Molecule 1: RNA (5'-R(\*GP\*GP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*CP\*GP\*AP\*CP\*CP\*GP\*AP\*UP\*CP\*C)-3')

Chain A:  11% 79% 11%



### 4.2.5 Score per residue for model 5

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

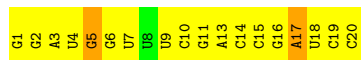
Chain A:  5% 79% 16%



### 4.2.6 Score per residue for model 6

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

Chain A:  5% 84% 11%



### 4.2.7 Score per residue for model 7

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



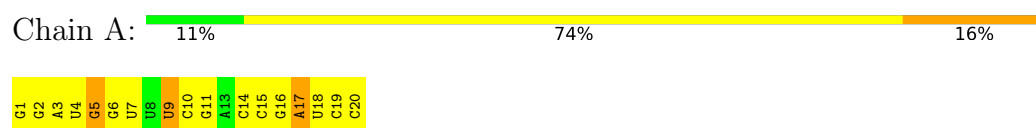
#### 4.2.8 Score per residue for model 8

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



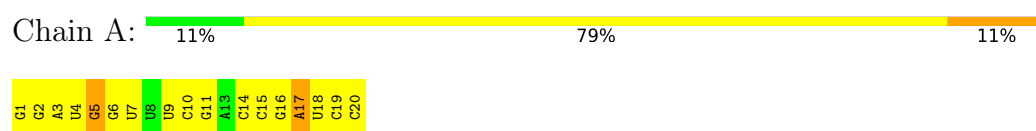
#### 4.2.9 Score per residue for model 9

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



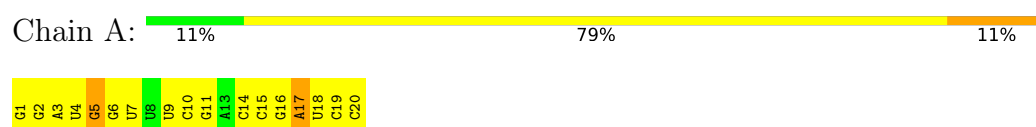
#### 4.2.10 Score per residue for model 10

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



#### 4.2.11 Score per residue for model 11

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



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *na*.

Of the 100 calculated structures, 11 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
CNS	structure calculation	1.3

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	90
Number of shifts mapped to atoms	90
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	20%



## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 53D

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	A	401	206	206	13±2
2	A	32	34	0	2±1
All	All	4763	2640	2266	152

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:C:H2'	1:A:15:C:C6	0.63	2.29	1	11
1:A:19:C:H2'	1:A:20:C:C6	0.62	2.29	1	11
1:A:6:G:H2'	1:A:7:U:C6	0.61	2.31	1	11
1:A:2:G:H2'	1:A:3:A:C8	0.59	2.32	1	11
2:A:101:53D:C24	2:A:101:53D:C28	0.57	2.82	1	1
1:A:19:C:H2'	1:A:20:C:H6	0.55	1.60	1	11
2:A:101:53D:O22	2:A:101:53D:C25	0.55	2.54	1	1
1:A:17:A:H2'	1:A:18:U:C6	0.54	2.37	1	11
1:A:3:A:H2'	1:A:4:U:C6	0.52	2.39	1	11
1:A:6:G:H2'	1:A:7:U:H6	0.51	1.62	1	11
1:A:1:G:H2'	1:A:2:G:C8	0.51	2.41	1	11

*Continued on next page...*

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:U:H5''	1:A:10:C:H5	0.50	1.67	3	1
1:A:9:U:H5''	1:A:10:C:C5	0.49	2.43	3	1
1:A:14:C:H2'	1:A:15:C:H6	0.48	1.67	1	11
1:A:9:U:H5'	1:A:10:C:C5	0.47	2.45	5	3
2:A:101:53D:C21	2:A:101:53D:C19	0.45	2.94	6	1
2:A:101:53D:C29	2:A:101:53D:C24	0.45	2.95	2	1
1:A:5:G:H2'	1:A:6:G:C8	0.45	2.47	11	11
1:A:7:U:H2'	1:A:8:U:C6	0.45	2.46	4	3
1:A:5:G:H1'	2:A:101:53D:O4	0.44	2.11	11	6
1:A:4:U:H3	1:A:17:A:H61	0.44	1.53	1	1
2:A:101:53D:C16	2:A:101:53D:C7	0.44	2.96	6	3
1:A:2:G:H2'	1:A:3:A:H8	0.43	1.71	1	1
1:A:9:U:H5'	1:A:10:C:H5	0.41	1.75	5	1
1:A:14:C:H6	1:A:14:C:O5'	0.41	1.98	1	1
2:A:101:53D:N14	2:A:101:53D:C20	0.41	2.84	9	1
2:A:101:53D:C7	2:A:101:53D:C16	0.41	2.99	7	1
1:A:5:G:H1'	2:A:101:53D:C4	0.40	2.45	3	1
2:A:101:53D:C20	2:A:101:53D:N14	0.40	2.84	10	1
1:A:19:C:H6	1:A:19:C:O5'	0.40	1.98	1	1
1:A:9:U:H6	1:A:9:U:O5'	0.40	1.98	1	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

### 6.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

### 6.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	18/19 (95%)	5±1 (30±4%)	0±0 (0±0%)	0.57±0.02
All	All	198/209 (95%)	60 (30%)	0 (0%)	0.57

The overall RNA backbone suiteness is 0.57.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	5	G	11
1	A	11	G	11
1	A	16	G	11
1	A	17	A	11
1	A	9	U	9
1	A	10	C	6
1	A	13	A	1

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	53D	A	101	-	35,35,35	1.46±0.01	3±0 (8±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	53D	A	101	-	50,50,50	1.89±0.01	7±0 (14±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	53D	A	101	-	-	0±0,21,33,33	0±0,4,4,4

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	101	53D	C15-N14	4.36	1.53	1.46	5	11
2	A	101	53D	C19-N14	4.35	1.53	1.46	4	11
2	A	101	53D	C8-N14	3.67	1.49	1.41	4	11

All 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
2	A	101	53D	C12-C11-N1	6.45	128.52	118.84	1	11
2	A	101	53D	C2-N1-C11	6.27	126.48	119.89	5	11
2	A	101	53D	C11-N1-C6	4.62	112.75	119.73	5	11
2	A	101	53D	C7-C8-C9	4.35	120.71	116.48	2	11
2	A	101	53D	C13-C11-N1	3.95	112.92	118.84	11	11
2	A	101	53D	C7-C8-N14	2.74	118.46	122.52	4	5
2	A	101	53D	C7-C2-N1	2.67	122.47	120.53	1	11
2	A	101	53D	C10-C9-C8	2.56	121.22	123.34	7	11

There are no chirality outliers.

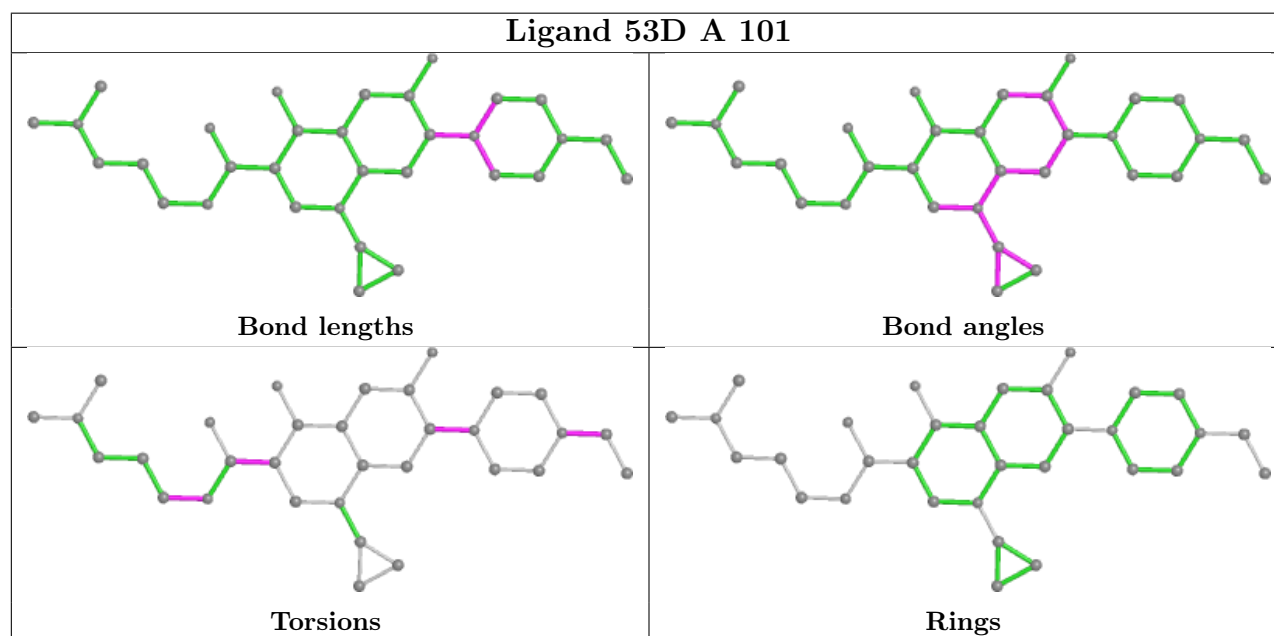
All unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	101	53D	O22-C22-C5-C4	10
2	A	101	53D	N23-C22-C5-C4	1

All unique ring outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	101	53D	C15-C16-C18-C19-N14-N17	4

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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 20% for the well-defined parts and 20% 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	90
Number of shifts mapped to atoms	90
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 20%, i.e. 70 atoms were assigned a chemical shift out of a possible 357. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Sugar	27/209 (13%)	27/114 (24%)	0/95 (0%)	0/0 (—%)
Base	43/148 (29%)	43/91 (47%)	0/32 (0%)	0/25 (0%)
Overall	70/357 (20%)	70/205 (34%)	0/127 (0%)	0/25 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 20%, i.e. 70 atoms were assigned a chemical shift out of a possible 357. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Sugar	27/209 (13%)	27/114 (24%)	0/95 (0%)	0/0 (—%)
Base	43/148 (29%)	43/91 (47%)	0/32 (0%)	0/25 (0%)
Overall	70/357 (20%)	70/205 (34%)	0/127 (0%)	0/25 (0%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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

### 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	107
Intra-residue ( $ i-j =0$ )	35
Sequential ( $ i-j =1$ )	22
Medium range ( $ i-j >1$ and $ i-j <5$ )	1
Long range ( $ i-j \geq 5$ )	19
Inter-chain	10
Hydrogen bond restraints	20
Disulfide bond restraints	0
Total dihedral-angle restraints	154
Number of unmapped restraints	0
Number of restraints per residue	13.1
Number of long range restraints per residue <sup>1</sup>	1.9

<sup>1</sup>Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

### 8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

#### 8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	2.0	0.2
0.2-0.5 (Medium)	2.0	0.27
>0.5 (Large)	None	None



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

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

## 9 Distance violation analysis ⓘ

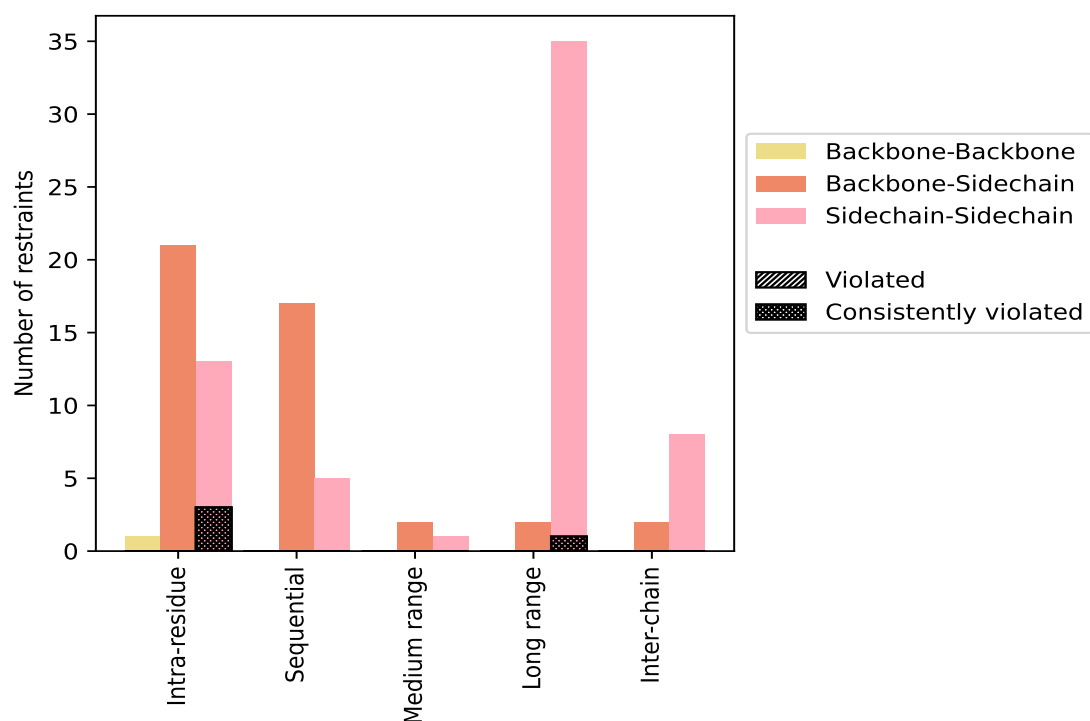
### 9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<a href="#">Intra-residue ( i-j =0)</a>	<a href="#">35</a>	<a href="#">32.7</a>	<a href="#">3</a>	<a href="#">8.6</a>	<a href="#">2.8</a>	<a href="#">3</a>	<a href="#">8.6</a>	<a href="#">2.8</a>
Backbone-Backbone	1	0.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	21	19.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	13	12.1	3	23.1	2.8	3	23.1	2.8
<a href="#">Sequential ( i-j =1)</a>	<a href="#">22</a>	<a href="#">20.6</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	17	15.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	5	4.7	0	0.0	0.0	0	0.0	0.0
<a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a>	<a href="#">1</a>	<a href="#">0.9</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1	0.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
<a href="#">Long range ( i-j ≥5)</a>	<a href="#">19</a>	<a href="#">17.8</a>	<a href="#">1</a>	<a href="#">5.3</a>	<a href="#">0.9</a>	<a href="#">1</a>	<a href="#">5.3</a>	<a href="#">0.9</a>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2	1.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	17	15.9	1	5.9	0.9	1	5.9	0.9
<a href="#">Inter-chain</a>	<a href="#">10</a>	<a href="#">9.3</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2	1.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	8	7.5	0	0.0	0.0	0	0.0	0.0
<a href="#">Hydrogen bond</a>	<a href="#">20</a>	<a href="#">18.7</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Disulfide bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Total</a>	<a href="#">107</a>	<a href="#">100.0</a>	<a href="#">4</a>	<a href="#">3.7</a>	<a href="#">3.7</a>	<a href="#">4</a>	<a href="#">3.7</a>	<a href="#">3.7</a>
Backbone-Backbone	1	0.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	44	41.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	62	57.9	4	6.5	3.7	4	6.5	3.7

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> violated in all the models

### 9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

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

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	3	0	0	1	0	4	0.22	0.27	0.06	0.24
2	3	0	0	1	0	4	0.22	0.27	0.05	0.24
3	3	0	0	1	0	4	0.22	0.27	0.05	0.24
4	3	0	0	1	0	4	0.22	0.27	0.05	0.24
5	3	0	0	1	0	4	0.22	0.27	0.05	0.24
6	3	0	0	1	0	4	0.22	0.27	0.05	0.24
7	3	0	0	1	0	4	0.22	0.27	0.05	0.24
8	3	0	0	1	0	4	0.22	0.27	0.05	0.24
9	3	0	0	1	0	4	0.22	0.27	0.05	0.24
10	3	0	0	1	0	4	0.22	0.27	0.05	0.24

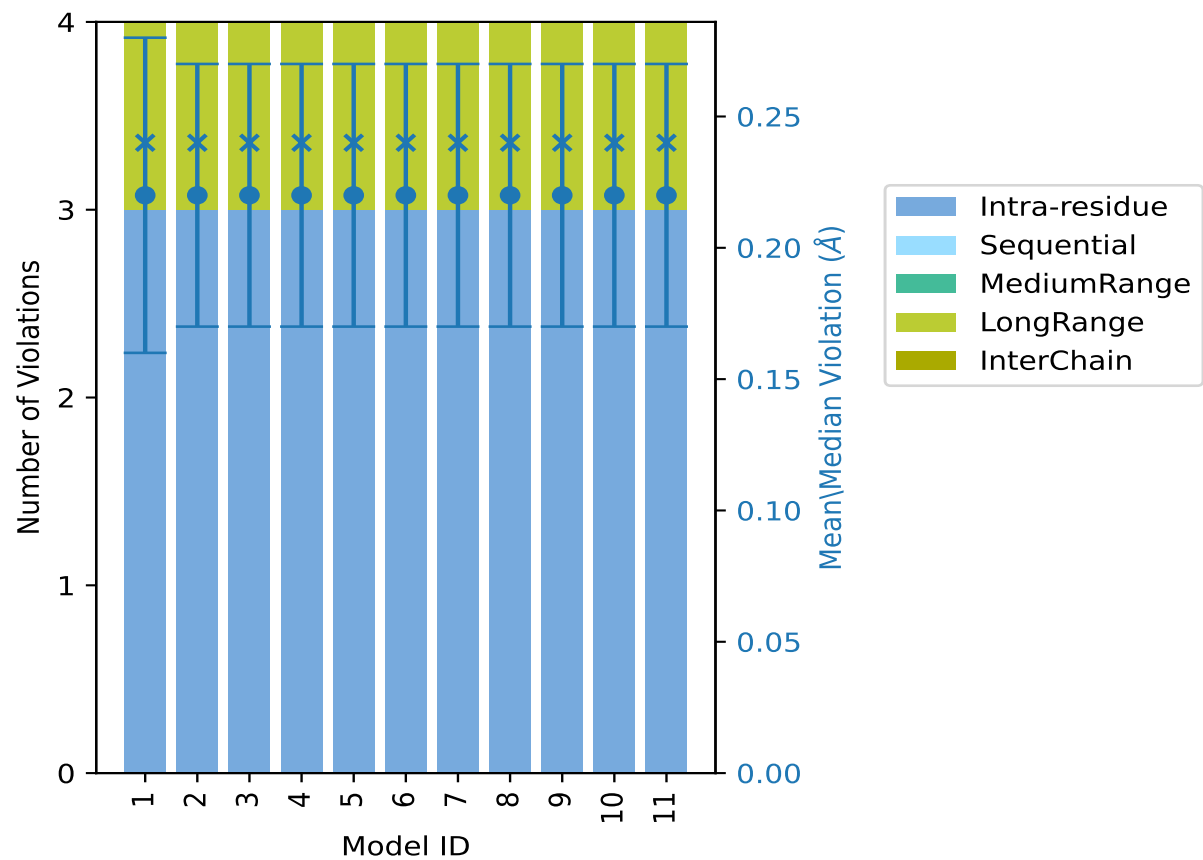
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	3	0	0	1	0	4	0.22	0.27	0.05	0.24

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble ⓘ

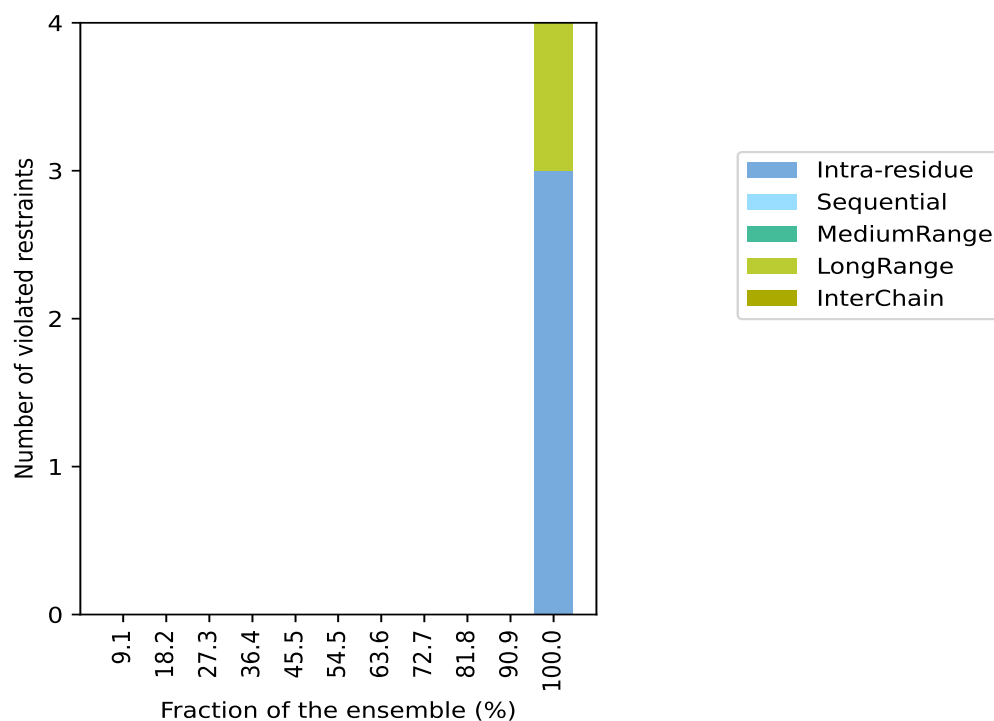
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 83(IR:32, SQ:22, MR:1, LR:18, IC:10) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	0	0	0	0	0	1	9.1
0	0	0	0	0	0	2	18.2
0	0	0	0	0	0	3	27.3
0	0	0	0	0	0	4	36.4
0	0	0	0	0	0	5	45.5
0	0	0	0	0	0	6	54.5
0	0	0	0	0	0	7	63.6
0	0	0	0	0	0	8	72.7
0	0	0	0	0	0	9	81.8
0	0	0	0	0	0	10	90.9
3	0	0	1	0	4	11	100.0

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

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

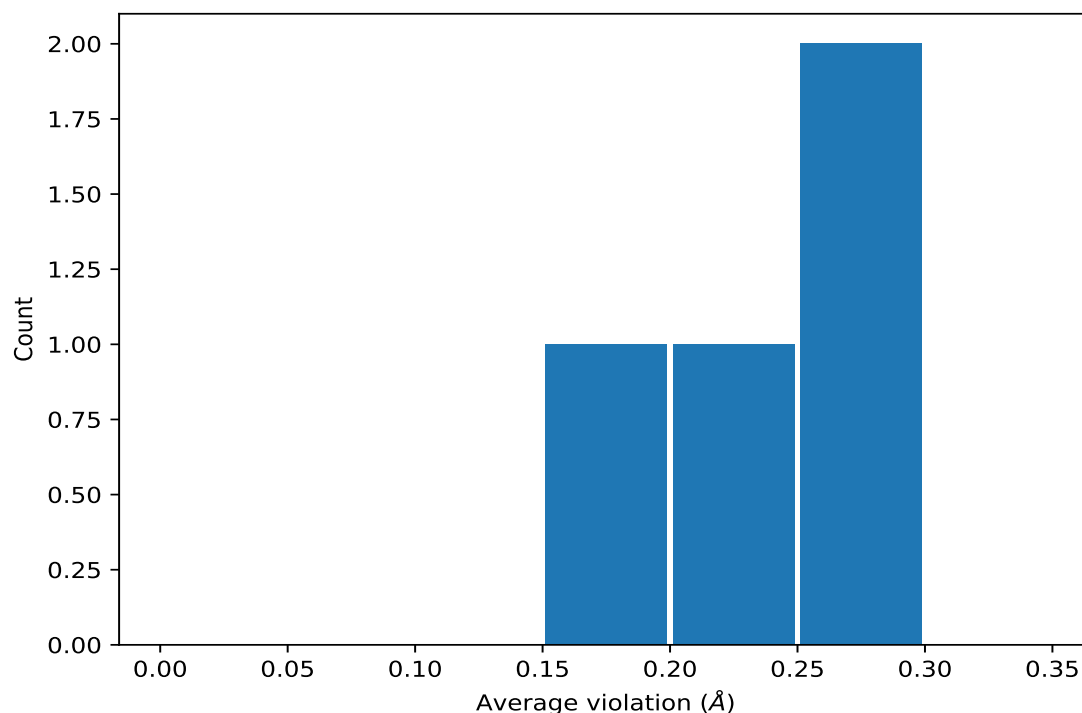
### 9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ



## 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.

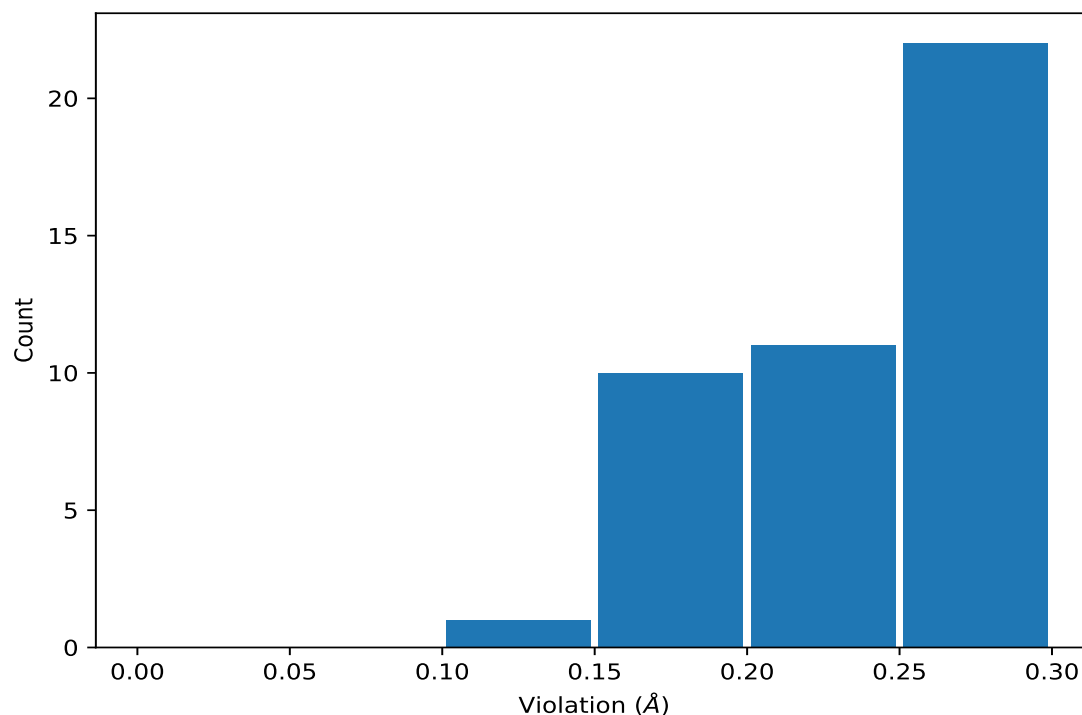
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,86)	2:101:A:53D:H131	2:101:A:53D:H132	11	0.27	0.0	0.27
(1,87)	2:101:A:53D:H132	2:101:A:53D:H131	11	0.27	0.0	0.27
(1,79)	2:101:A:53D:H132	2:101:A:53D:H6	11	0.2	0.0	0.2
(1,68)	1:19:A:C:H42	1:2:A:G:H1	11	0.15	0.01	0.15

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

## 9.5 All violated distance restraints [i](#)

### 9.5.1 Histogram : Distribution of distance violations [i](#)

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



### 9.5.2 Table : All distance violations [i](#)

The following table 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)
(1,87)	2:101:A:53D:H132	2:101:A:53D:H131	1	0.27
(1,87)	2:101:A:53D:H132	2:101:A:53D:H131	2	0.27
(1,87)	2:101:A:53D:H132	2:101:A:53D:H131	3	0.27
(1,87)	2:101:A:53D:H132	2:101:A:53D:H131	4	0.27
(1,87)	2:101:A:53D:H132	2:101:A:53D:H131	5	0.27
(1,87)	2:101:A:53D:H132	2:101:A:53D:H131	6	0.27
(1,87)	2:101:A:53D:H132	2:101:A:53D:H131	7	0.27
(1,87)	2:101:A:53D:H132	2:101:A:53D:H131	8	0.27
(1,87)	2:101:A:53D:H132	2:101:A:53D:H131	9	0.27
(1,87)	2:101:A:53D:H132	2:101:A:53D:H131	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	2:101:A:53D:H132	2:101:A:53D:H131	11	0.27
(1,86)	2:101:A:53D:H131	2:101:A:53D:H132	1	0.27
(1,86)	2:101:A:53D:H131	2:101:A:53D:H132	2	0.27
(1,86)	2:101:A:53D:H131	2:101:A:53D:H132	3	0.27
(1,86)	2:101:A:53D:H131	2:101:A:53D:H132	4	0.27
(1,86)	2:101:A:53D:H131	2:101:A:53D:H132	5	0.27
(1,86)	2:101:A:53D:H131	2:101:A:53D:H132	6	0.27
(1,86)	2:101:A:53D:H131	2:101:A:53D:H132	7	0.27
(1,86)	2:101:A:53D:H131	2:101:A:53D:H132	8	0.27
(1,86)	2:101:A:53D:H131	2:101:A:53D:H132	9	0.27
(1,86)	2:101:A:53D:H131	2:101:A:53D:H132	10	0.27
(1,86)	2:101:A:53D:H131	2:101:A:53D:H132	11	0.27
(1,79)	2:101:A:53D:H132	2:101:A:53D:H6	1	0.2
(1,79)	2:101:A:53D:H132	2:101:A:53D:H6	2	0.2
(1,79)	2:101:A:53D:H132	2:101:A:53D:H6	3	0.2
(1,79)	2:101:A:53D:H132	2:101:A:53D:H6	4	0.2
(1,79)	2:101:A:53D:H132	2:101:A:53D:H6	5	0.2
(1,79)	2:101:A:53D:H132	2:101:A:53D:H6	6	0.2
(1,79)	2:101:A:53D:H132	2:101:A:53D:H6	7	0.2
(1,79)	2:101:A:53D:H132	2:101:A:53D:H6	8	0.2
(1,79)	2:101:A:53D:H132	2:101:A:53D:H6	9	0.2
(1,79)	2:101:A:53D:H132	2:101:A:53D:H6	10	0.2
(1,79)	2:101:A:53D:H132	2:101:A:53D:H6	11	0.2
(1,68)	1:19:A:C:H42	1:2:A:G:H1	2	0.15
(1,68)	1:19:A:C:H42	1:2:A:G:H1	3	0.15
(1,68)	1:19:A:C:H42	1:2:A:G:H1	4	0.15
(1,68)	1:19:A:C:H42	1:2:A:G:H1	5	0.15
(1,68)	1:19:A:C:H42	1:2:A:G:H1	6	0.15
(1,68)	1:19:A:C:H42	1:2:A:G:H1	7	0.15
(1,68)	1:19:A:C:H42	1:2:A:G:H1	8	0.15
(1,68)	1:19:A:C:H42	1:2:A:G:H1	9	0.15
(1,68)	1:19:A:C:H42	1:2:A:G:H1	10	0.15
(1,68)	1:19:A:C:H42	1:2:A:G:H1	11	0.15
(1,68)	1:19:A:C:H42	1:2:A:G:H1	1	0.12



## 10 Dihedral-angle violation analysis ⓘ

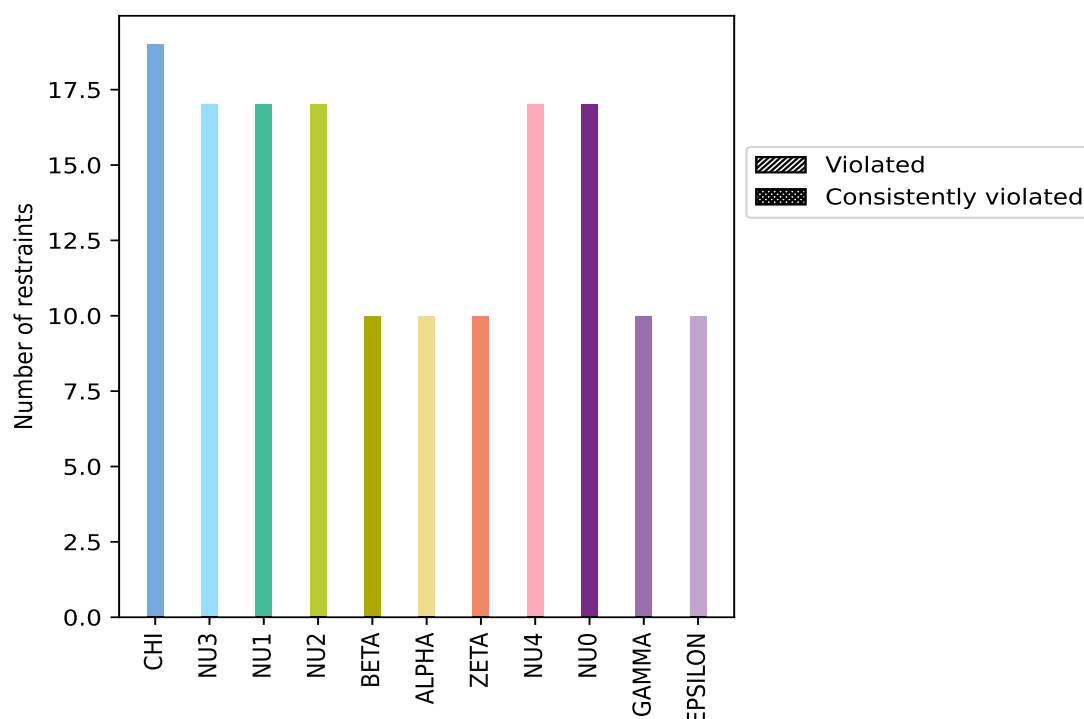
### 10.1 Summary of dihedral-angle violations ⓘ

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	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
CHI	19	12.3	0	0.0	0.0	0	0.0	0.0
NU3	17	11.0	0	0.0	0.0	0	0.0	0.0
NU1	17	11.0	0	0.0	0.0	0	0.0	0.0
NU2	17	11.0	0	0.0	0.0	0	0.0	0.0
BETA	10	6.5	0	0.0	0.0	0	0.0	0.0
ALPHA	10	6.5	0	0.0	0.0	0	0.0	0.0
ZETA	10	6.5	0	0.0	0.0	0	0.0	0.0
NU4	17	11.0	0	0.0	0.0	0	0.0	0.0
NU0	17	11.0	0	0.0	0.0	0	0.0	0.0
GAMMA	10	6.5	0	0.0	0.0	0	0.0	0.0
EPSILON	10	6.5	0	0.0	0.0	0	0.0	0.0
Total	154	100.0	0	0.0	0.0	0	0.0	0.0

<sup>1</sup> percentage calculated with respect to total number of dihedral-angle restraints, <sup>2</sup> percentage calculated with respect to number of restraints in a particular dihedral-angle type, <sup>3</sup> violated in at least one model, <sup>4</sup> 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