



# wwPDB NMR Structure Validation Summary Report ⓘ

May 28, 2026 – 09:21 AM EDT

PDB ID : 8XC7 / pdb\_00008xc7  
BMRB ID : 36621  
Title : Structure of LL-D49194-alpha-1 covalently bound to guanosine-2'-fluorinated d(AACCGGTT)2  
Authors : Gao, R.Q.; Tang, G.L.; Cao, C.  
Deposited on : 2023-12-08

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

We welcome your comments at [validation@mail.wwpdb.org](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 : **FAILED**  
Mogul : 2022.3.0, CSD as543be (2022)  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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 23%.

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 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.

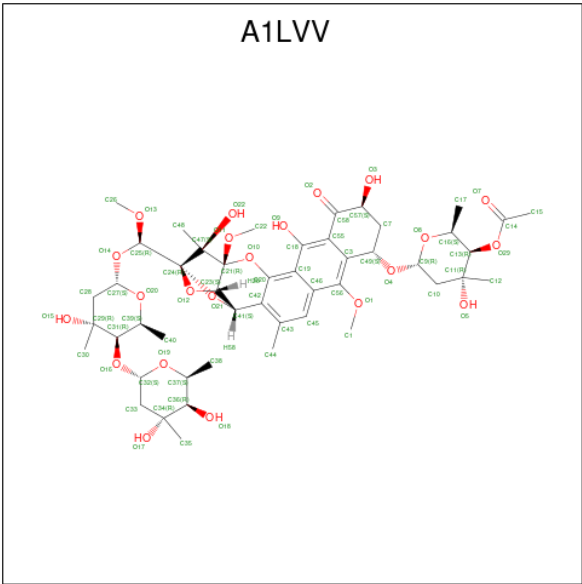
3 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 776 atoms, of which 310 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called DNA (5'-D(\*AP\*AP\*CP\*CP\*2''F-GP\*2''F-GP\*TP\*T)-3').

| Mol | Chain | Residues | Atoms |    |   |    |    |    |   | Trace |
|-----|-------|----------|-------|----|---|----|----|----|---|-------|
| 1   | A     | 8        | Total | C  | F | H  | N  | O  | P | 0     |
|     |       |          | 253   | 78 | 2 | 90 | 30 | 46 | 7 |       |
| 1   | B     | 8        | Total | C  | F | H  | N  | O  | P | 0     |
|     |       |          | 253   | 78 | 2 | 90 | 30 | 46 | 7 |       |

- Molecule 2 is LL-D49194alpha1 (CCD ID: A1LVV) (formula: C<sub>48</sub>H<sub>66</sub>O<sub>22</sub>) (labeled as "Ligand of Interest" by depositor).



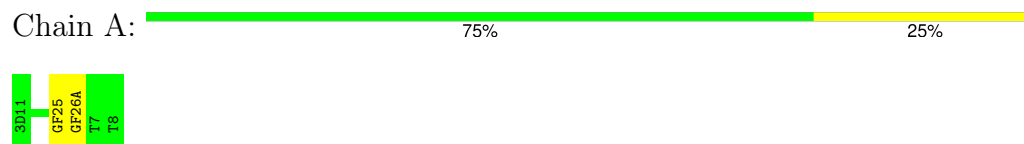
| Mol | Chain | Residues | Atoms |    |    |    |
|-----|-------|----------|-------|----|----|----|
| 2   | A     | 1        | Total | C  | H  | O  |
|     |       |          | 135   | 48 | 65 | 22 |
| 2   | B     | 1        | Total | C  | H  | O  |
|     |       |          | 135   | 48 | 65 | 22 |

## 4 Residue-property plots [i](#)

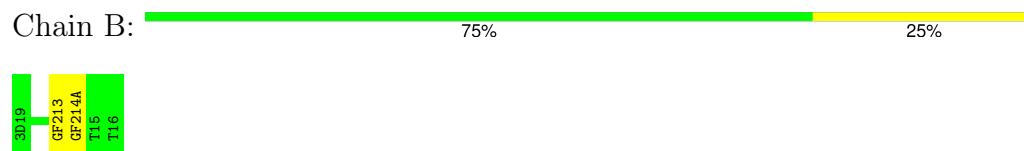
### 4.1 Average score per residue in the NMR ensemble

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(\*AP\*AP\*CP\*CP\*2''F-GP\*2''F-GP\*TP\*T)-3')



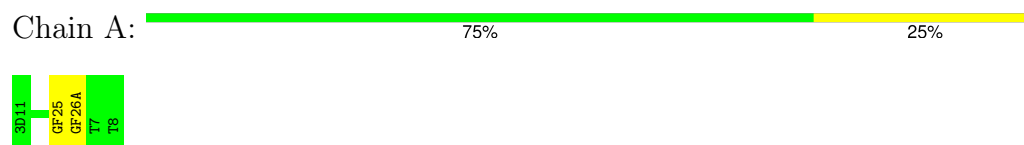
- Molecule 1: DNA (5'-D(\*AP\*AP\*CP\*CP\*2''F-GP\*2''F-GP\*TP\*T)-3')



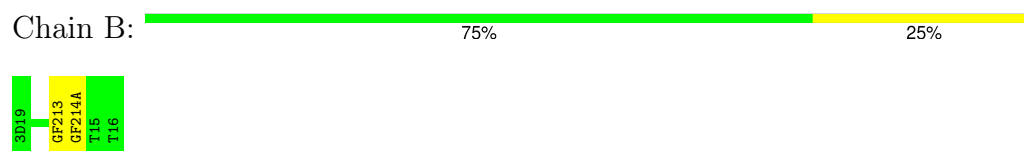
### 4.2 Residue scores for the representative (author defined) model from the NMR ensemble

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

- Molecule 1: DNA (5'-D(\*AP\*AP\*CP\*CP\*2''F-GP\*2''F-GP\*TP\*T)-3')



- Molecule 1: DNA (5'-D(\*AP\*AP\*CP\*CP\*2''F-GP\*2''F-GP\*TP\*T)-3')



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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                       | 98             |
| Number of shifts mapped to atoms             | 77             |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 21             |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 23%            |

## 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 23% for the well-defined parts and 23% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

#### 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                  | 98 |
| Number of shifts mapped to atoms        | 77 |
| Number of unparsed shifts               | 0  |
| Number of shifts with mapping errors    | 21 |
| Number of shifts with mapping warnings  | 0  |
| Number of shift outliers (ShiftChecker) | 0  |

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 21) occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 6   | GF2  | H30  | 3.634      | .           | .         |
| 1       | A     | 6   | GF2  | H33  | 5.469      | .           | .         |
| 1       | A     | 6   | GF2  | H34  | 2.067      | .           | .         |
| 1       | A     | 6   | GF2  | H35  | 2.117      | .           | .         |
| 1       | A     | 6   | GF2  | H36  | 1.422      | .           | .         |
| 1       | A     | 6   | GF2  | H40  | 3.356      | .           | .         |
| 1       | A     | 6   | GF2  | H41  | 5.081      | .           | .         |
| 1       | A     | 6   | GF2  | H42  | 2.006      | .           | .         |
| 1       | A     | 6   | GF2  | H44  | 1.271      | .           | .         |
| 1       | A     | 6   | GF2  | H50  | 4.549      | .           | .         |
| 1       | A     | 6   | GF2  | H51  | 1.248      | .           | .         |
| 1       | A     | 6   | GF2  | H54  | 4.733      | .           | .         |
| 1       | A     | 6   | GF2  | H55  | 1.248      | .           | .         |
| 1       | A     | 6   | GF2  | H59  | 2.12       | .           | .         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 6   | GF2  | H6   | 1.918      | .           | .         |
| 1       | A     | 6   | GF2  | H62  | 6.692      | .           | .         |
| 1       | A     | 6   | GF2  | H64  | 4.903      | .           | .         |
| 1       | A     | 6   | GF2  | H65  | 5.11       | .           | .         |
| 1       | A     | 6   | GF2  | H66  | 5.222      | .           | .         |
| 1       | A     | 6   | GF2  | H7   | 2.905      | .           | .         |
| 1       | A     | 6   | GF2  | H9   | 5.365      | .           | .         |

### 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 23%, i.e. 45 atoms were assigned a chemical shift out of a possible 192. 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   | 34/120 (28%) | 34/70 (49%)    | 0/50 (0%)       | 0/0 (—%)        |
| Base    | 11/72 (15%)  | 11/42 (26%)    | 0/20 (0%)       | 0/10 (0%)       |
| Overall | 45/192 (23%) | 45/112 (40%)   | 0/70 (0%)       | 0/10 (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                                | 448   |
| Intra-residue ( $ i-j =0$ )                              | 250   |
| Sequential ( $ i-j =1$ )                                 | 82    |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 10    |
| Long range ( $ i-j \geq 5$ )                             | 0     |
| Inter-chain                                              | 60    |
| Hydrogen bond restraints                                 | 46    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 66    |
| Number of unmapped restraints                            | 150   |
| Number of restraints per residue                         | 28.6  |
| Number of long range restraints per residue <sup>1</sup> | 0.0   |

<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)  | 17.6                                   | 0.2     |
| 0.2-0.5 (Medium) | 7.8                                    | 0.34    |
| >0.5 (Large)     | 14.0                                   | 7.49    |

### 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)   | 3.1                                    | 2.6     |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

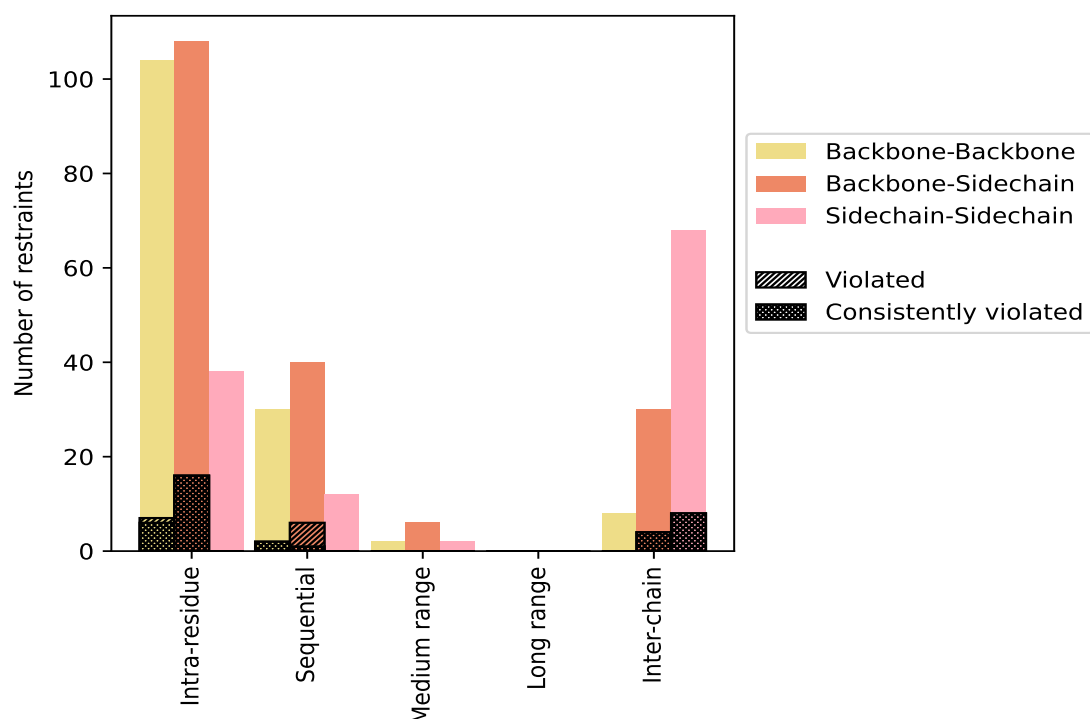
### 9.1 Summary of distance violations ⓘ

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> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>250</b> | <b>55.8</b>    | <b>23</b>             | <b>9.2</b>     | <b>5.1</b>     | <b>22</b>                          | <b>8.8</b>     | <b>4.9</b>     |
| Backbone-Backbone                                                           | 104        | 23.2           | 7                     | 6.7            | 1.6            | 6                                  | 5.8            | 1.3            |
| Backbone-Sidechain                                                          | 108        | 24.1           | 16                    | 14.8           | 3.6            | 16                                 | 14.8           | 3.6            |
| Sidechain-Sidechain                                                         | 38         | 8.5            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>82</b>  | <b>18.3</b>    | <b>8</b>              | <b>9.8</b>     | <b>1.8</b>     | <b>3</b>                           | <b>3.7</b>     | <b>0.7</b>     |
| Backbone-Backbone                                                           | 30         | 6.7            | 2                     | 6.7            | 0.4            | 2                                  | 6.7            | 0.4            |
| Backbone-Sidechain                                                          | 40         | 8.9            | 6                     | 15.0           | 1.3            | 1                                  | 2.5            | 0.2            |
| Sidechain-Sidechain                                                         | 12         | 2.7            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>10</b>  | <b>2.2</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 2          | 0.4            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 6          | 1.3            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 2          | 0.4            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| 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            |
| <b>Inter-chain</b>                                                          | <b>60</b>  | <b>13.4</b>    | <b>8</b>              | <b>13.3</b>    | <b>1.8</b>     | <b>8</b>                           | <b>13.3</b>    | <b>1.8</b>     |
| Backbone-Backbone                                                           | 8          | 1.8            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 26         | 5.8            | 2                     | 7.7            | 0.4            | 2                                  | 7.7            | 0.4            |
| Sidechain-Sidechain                                                         | 26         | 5.8            | 6                     | 23.1           | 1.3            | 6                                  | 23.1           | 1.3            |
| <b>Hydrogen bond</b>                                                        | <b>46</b>  | <b>10.3</b>    | <b>4</b>              | <b>8.7</b>     | <b>0.9</b>     | <b>4</b>                           | <b>8.7</b>     | <b>0.9</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>448</b> | <b>100.0</b>   | <b>43</b>             | <b>9.6</b>     | <b>9.6</b>     | <b>37</b>                          | <b>8.3</b>     | <b>8.3</b>     |
| Backbone-Backbone                                                           | 144        | 32.1           | 9                     | 6.2            | 2.0            | 8                                  | 5.6            | 1.8            |
| Backbone-Sidechain                                                          | 184        | 41.1           | 26                    | 14.1           | 5.8            | 21                                 | 11.4           | 4.7            |
| Sidechain-Sidechain                                                         | 120        | 26.8           | 8                     | 6.7            | 1.8            | 8                                  | 6.7            | 1.8            |

<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 disulfid 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        | 22                   | 5               | 0               | 0               | 12              | 39    | 1.56     | 7.45    | 2.23                | 0.22       |
| 2        | 23                   | 5               | 0               | 0               | 12              | 40    | 1.51     | 7.44    | 2.21                | 0.22       |
| 3        | 23                   | 6               | 0               | 0               | 12              | 41    | 1.48     | 7.49    | 2.2                 | 0.22       |
| 4        | 23                   | 6               | 0               | 0               | 12              | 41    | 1.49     | 7.41    | 2.19                | 0.22       |
| 5        | 22                   | 5               | 0               | 0               | 12              | 39    | 1.55     | 7.46    | 2.23                | 0.23       |
| 6        | 23                   | 5               | 0               | 0               | 12              | 40    | 1.52     | 7.42    | 2.21                | 0.23       |
| 7        | 23                   | 5               | 0               | 0               | 12              | 40    | 1.52     | 7.41    | 2.21                | 0.22       |
| 8        | 22                   | 6               | 0               | 0               | 12              | 40    | 1.52     | 7.49    | 2.21                | 0.23       |
| 9        | 22                   | 5               | 0               | 0               | 12              | 39    | 1.55     | 7.45    | 2.22                | 0.23       |
| 10       | 23                   | 5               | 0               | 0               | 12              | 40    | 1.52     | 7.42    | 2.21                | 0.23       |

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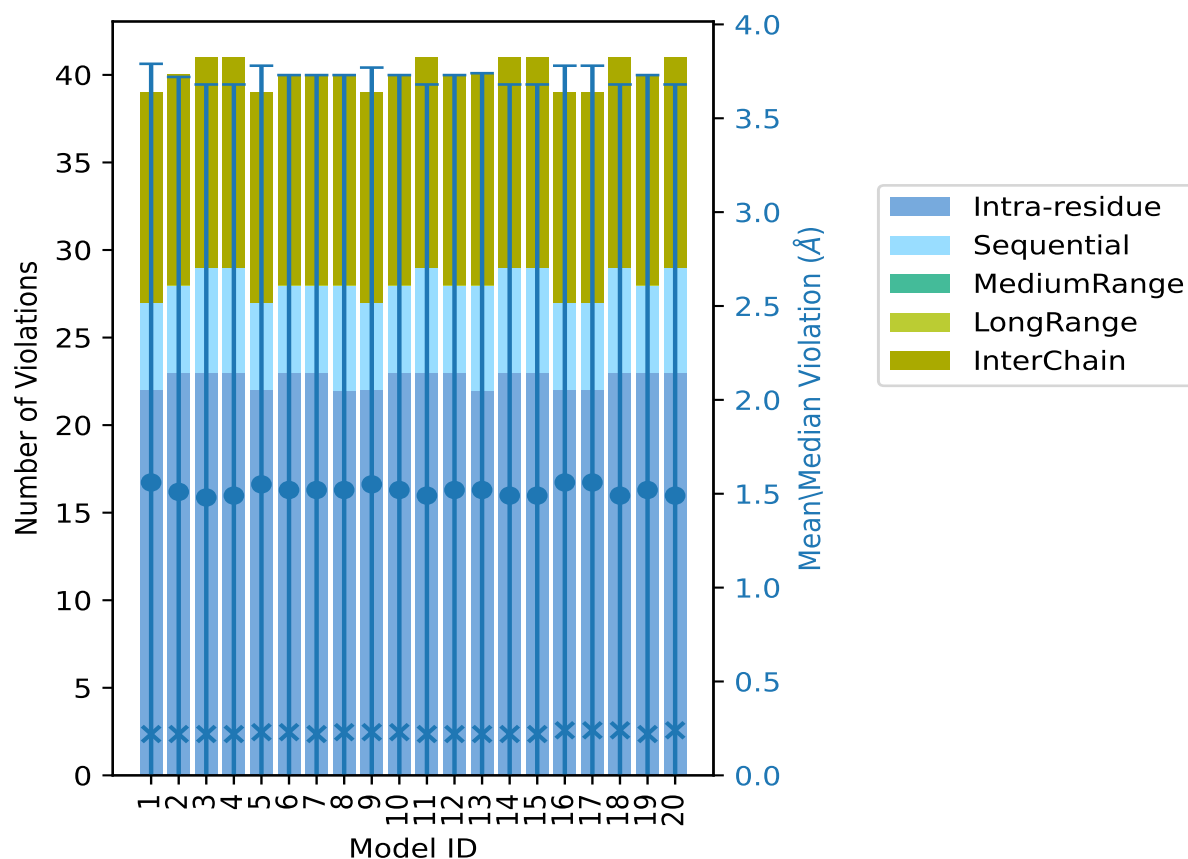
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 23                   | 6               | 0               | 0               | 12              | 41    | 1.49     | 7.43    | 2.19                | 0.22       |
| 12       | 23                   | 5               | 0               | 0               | 12              | 40    | 1.52     | 7.44    | 2.21                | 0.22       |
| 13       | 22                   | 6               | 0               | 0               | 12              | 40    | 1.52     | 7.47    | 2.22                | 0.22       |
| 14       | 23                   | 6               | 0               | 0               | 12              | 41    | 1.49     | 7.44    | 2.19                | 0.22       |
| 15       | 23                   | 6               | 0               | 0               | 12              | 41    | 1.49     | 7.45    | 2.19                | 0.22       |
| 16       | 22                   | 5               | 0               | 0               | 12              | 39    | 1.56     | 7.45    | 2.22                | 0.24       |
| 17       | 22                   | 5               | 0               | 0               | 12              | 39    | 1.56     | 7.47    | 2.22                | 0.24       |
| 18       | 23                   | 6               | 0               | 0               | 12              | 41    | 1.49     | 7.45    | 2.19                | 0.24       |
| 19       | 23                   | 5               | 0               | 0               | 12              | 40    | 1.52     | 7.44    | 2.21                | 0.22       |
| 20       | 23                   | 6               | 0               | 0               | 12              | 41    | 1.49     | 7.44    | 2.19                | 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, 363(IR:227, SQ:74, MR:10, LR:0, IC:52) restraints are not violated in the ensemble.

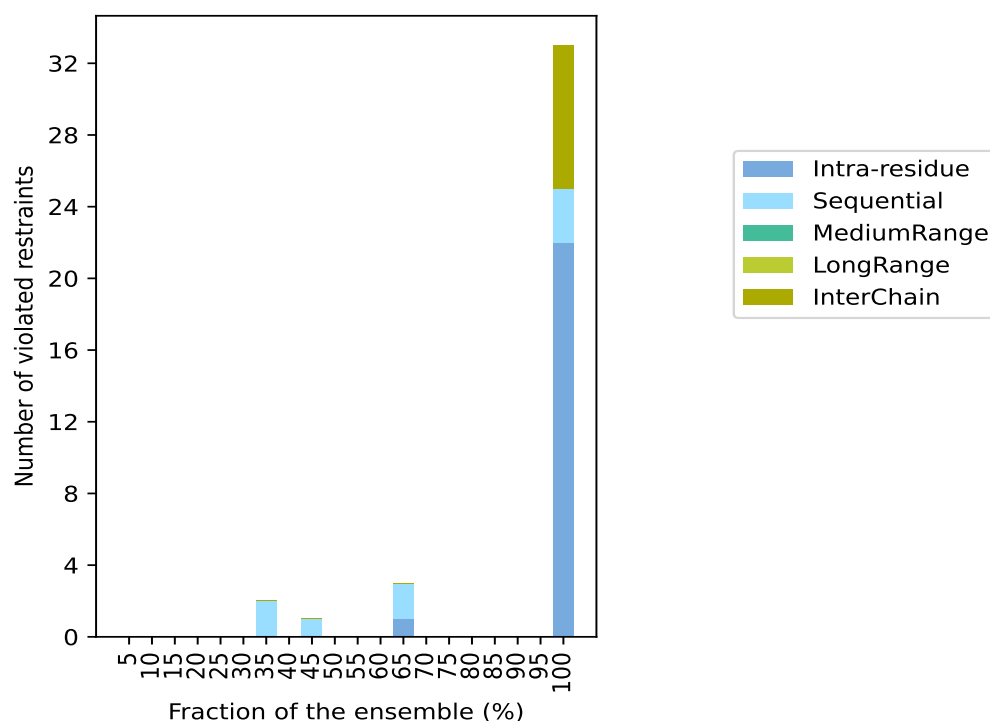
| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <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                        | 5.0   |
| 0                             | 0               | 0               | 0               | 0               | 0     | 2                        | 10.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 3                        | 15.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 4                        | 20.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 5                        | 25.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 6                        | 30.0  |
| 0                             | 2               | 0               | 0               | 0               | 2     | 7                        | 35.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 8                        | 40.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 9                        | 45.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 10                       | 50.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 11                       | 55.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 12                       | 60.0  |
| 1                             | 2               | 0               | 0               | 0               | 3     | 13                       | 65.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 14                       | 70.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 15                       | 75.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 16                       | 80.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 17                       | 85.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 18                       | 90.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 19                       | 95.0  |
| 22                            | 3               | 0               | 0               | 8               | 33    | 20                       | 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



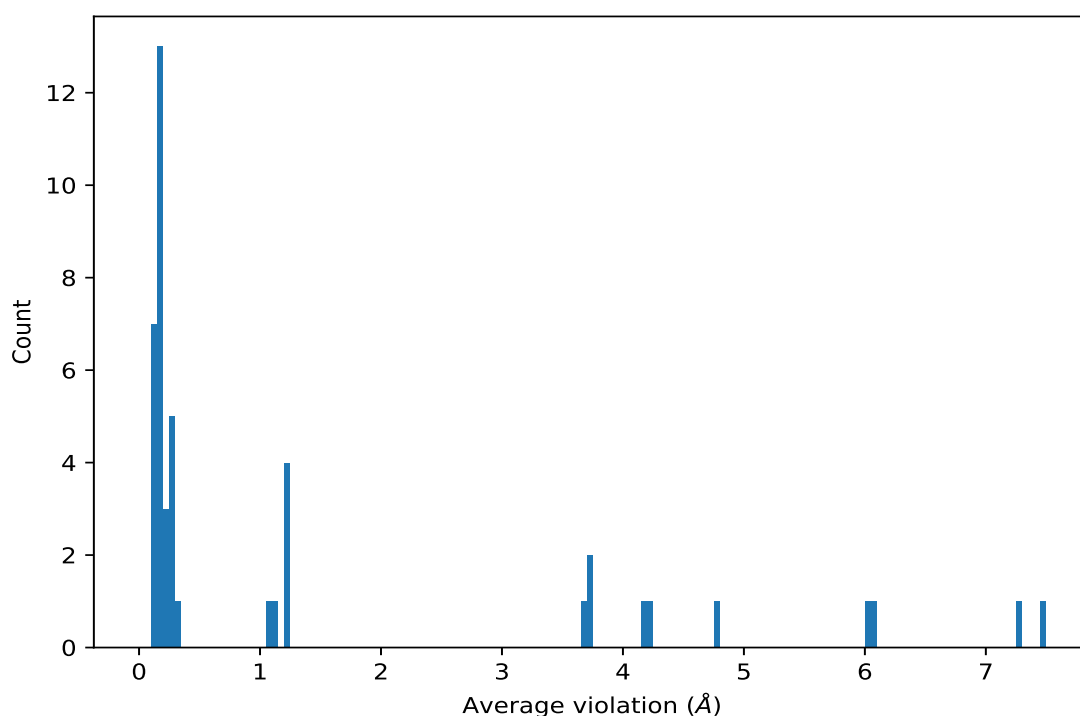
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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 violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

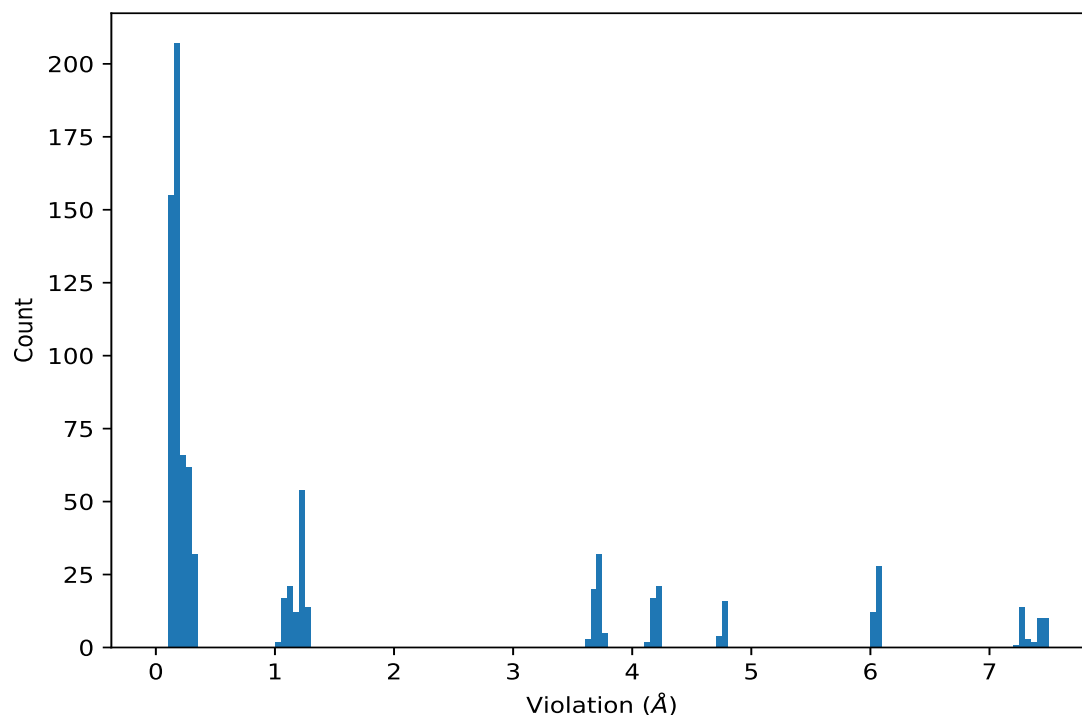
| Key     | Atom-1         | Atom-2        | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|----------------|---------------|---------------------|----------|---------------------|------------|
| (1,13)  | 1:13:B:GF2:H2' | 1:4:A:DC:O2   | 20                  | 7.45     | 0.02                | 7.44       |
| (1,27)  | 1:5:A:GF2:H2'  | 1:12:B:DC:O2  | 20                  | 7.29     | 0.04                | 7.27       |
| (1,9)   | 1:13:B:GF2:H8  | 1:4:A:DC:N3   | 20                  | 6.06     | 0.01                | 6.06       |
| (1,23)  | 1:5:A:GF2:H8   | 1:12:B:DC:N3  | 20                  | 6.05     | 0.01                | 6.05       |
| (4,193) | 1:4:A:DC:H5    | 1:13:B:GF2:H8 | 20                  | 4.76     | 0.01                | 4.76       |
| (4,183) | 1:4:A:DC:H41   | 1:13:B:GF2:H8 | 20                  | 4.22     | 0.02                | 4.23       |
| (4,184) | 1:12:B:DC:H41  | 1:5:A:GF2:H8  | 20                  | 4.18     | 0.02                | 4.17       |
| (4,224) | 1:13:B:GF2:H8  | 1:4:A:DC:H42  | 20                  | 3.73     | 0.02                | 3.74       |
| (4,194) | 1:12:B:DC:H5   | 1:5:A:GF2:H8  | 20                  | 3.71     | 0.02                | 3.71       |
| (4,223) | 1:5:A:GF2:H8   | 1:12:B:DC:H42 | 20                  | 3.67     | 0.02                | 3.67       |

<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 provides the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key    | Atom-1         | Atom-2      | Model ID | Violation (Å) |
|--------|----------------|-------------|----------|---------------|
| (1,13) | 1:13:B:GF2:H2' | 1:4:A:DC:O2 | 3        | 7.49          |
| (1,13) | 1:13:B:GF2:H2' | 1:4:A:DC:O2 | 8        | 7.49          |
| (1,13) | 1:13:B:GF2:H2' | 1:4:A:DC:O2 | 13       | 7.47          |
| (1,13) | 1:13:B:GF2:H2' | 1:4:A:DC:O2 | 17       | 7.47          |
| (1,13) | 1:13:B:GF2:H2' | 1:4:A:DC:O2 | 5        | 7.46          |
| (1,13) | 1:13:B:GF2:H2' | 1:4:A:DC:O2 | 1        | 7.45          |
| (1,13) | 1:13:B:GF2:H2' | 1:4:A:DC:O2 | 9        | 7.45          |
| (1,13) | 1:13:B:GF2:H2' | 1:4:A:DC:O2 | 15       | 7.45          |
| (1,13) | 1:13:B:GF2:H2' | 1:4:A:DC:O2 | 16       | 7.45          |
| (1,13) | 1:13:B:GF2:H2' | 1:4:A:DC:O2 | 18       | 7.45          |

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

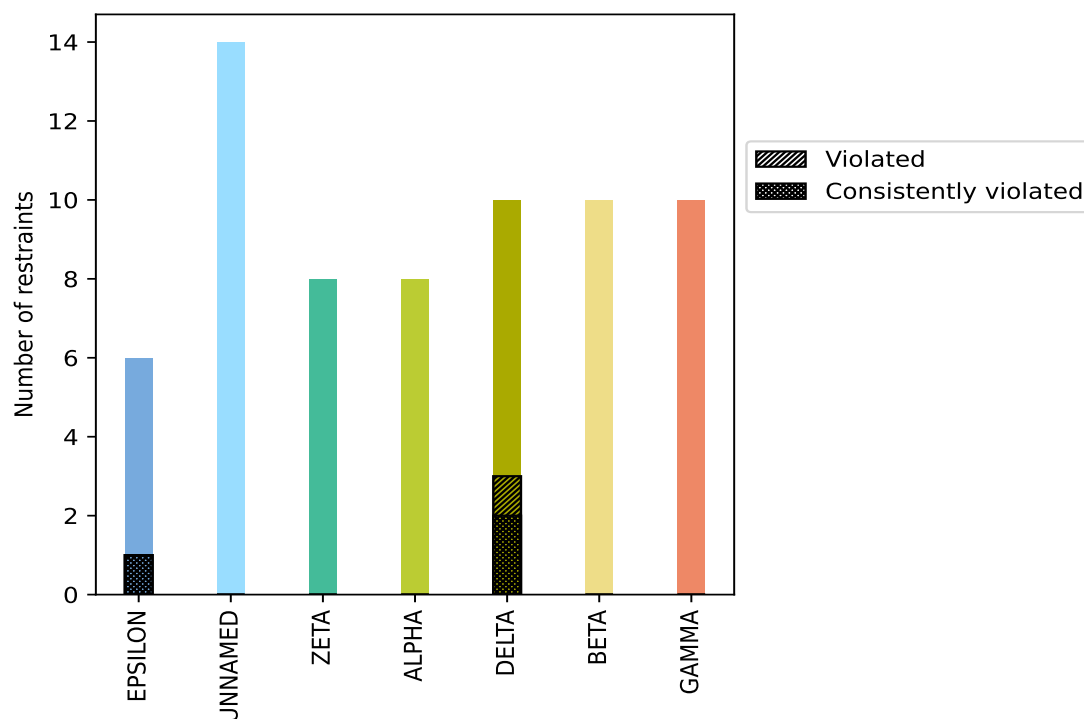
### 10.1 Summary of dihedral-angle violations [i](#)

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 | % <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> |
| EPSILON    | 6     | 9.1            | 1                     | 16.7           | 1.5            | 1                                  | 16.7           | 1.5            |
| UNNAMED    | 14    | 21.2           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| ZETA       | 8     | 12.1           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| ALPHA      | 8     | 12.1           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| DELTA      | 10    | 15.2           | 3                     | 30.0           | 4.5            | 2                                  | 20.0           | 3.0            |
| BETA       | 10    | 15.2           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| GAMMA      | 10    | 15.2           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Total      | 66    | 100.0          | 4                     | 6.1            | 6.1            | 3                                  | 4.5            | 4.5            |

<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](#)



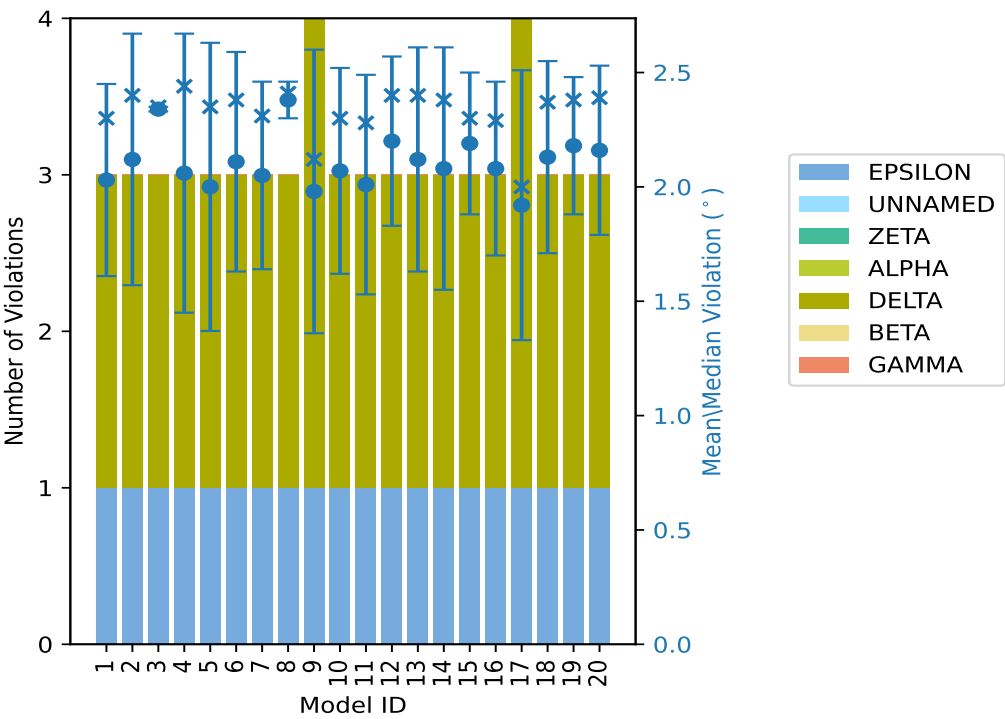
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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 |         |      |       |       |      |       |   | Total | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|---------|------|-------|-------|------|-------|---|-------|----------|---------|--------|------------|
|          | EPSILON              | UNNAMED | ZETA | ALPHA | DELTA | BETA | GAMMA |   |       |          |         |        |            |
| 1        | 1                    | 0       | 0    | 0     | 2     | 0    | 0     | 3 | 2.03  | 2.35     | 0.42    | 2.3    |            |
| 2        | 1                    | 0       | 0    | 0     | 2     | 0    | 0     | 3 | 2.12  | 2.6      | 0.55    | 2.4    |            |
| 3        | 1                    | 0       | 0    | 0     | 2     | 0    | 0     | 3 | 2.34  | 2.35     | 0.01    | 2.35   |            |
| 4        | 1                    | 0       | 0    | 0     | 2     | 0    | 0     | 3 | 2.06  | 2.54     | 0.61    | 2.44   |            |
| 5        | 1                    | 0       | 0    | 0     | 2     | 0    | 0     | 3 | 2.0   | 2.54     | 0.63    | 2.35   |            |
| 6        | 1                    | 0       | 0    | 0     | 2     | 0    | 0     | 3 | 2.11  | 2.52     | 0.48    | 2.38   |            |
| 7        | 1                    | 0       | 0    | 0     | 2     | 0    | 0     | 3 | 2.05  | 2.37     | 0.41    | 2.31   |            |
| 8        | 1                    | 0       | 0    | 0     | 2     | 0    | 0     | 3 | 2.38  | 2.46     | 0.08    | 2.41   |            |
| 9        | 1                    | 0       | 0    | 0     | 3     | 0    | 0     | 4 | 1.98  | 2.6      | 0.62    | 2.12   |            |
| 10       | 1                    | 0       | 0    | 0     | 2     | 0    | 0     | 3 | 2.07  | 2.46     | 0.45    | 2.3    |            |
| 11       | 1                    | 0       | 0    | 0     | 2     | 0    | 0     | 3 | 2.01  | 2.42     | 0.48    | 2.28   |            |
| 12       | 1                    | 0       | 0    | 0     | 2     | 0    | 0     | 3 | 2.2   | 2.51     | 0.37    | 2.4    |            |
| 13       | 1                    | 0       | 0    | 0     | 2     | 0    | 0     | 3 | 2.12  | 2.54     | 0.49    | 2.4    |            |
| 14       | 1                    | 0       | 0    | 0     | 2     | 0    | 0     | 3 | 2.08  | 2.53     | 0.53    | 2.38   |            |
| 15       | 1                    | 0       | 0    | 0     | 2     | 0    | 0     | 3 | 2.19  | 2.5      | 0.31    | 2.3    |            |
| 16       | 1                    | 0       | 0    | 0     | 2     | 0    | 0     | 3 | 2.08  | 2.41     | 0.38    | 2.29   |            |
| 17       | 1                    | 0       | 0    | 0     | 3     | 0    | 0     | 4 | 1.92  | 2.53     | 0.59    | 2.0    |            |
| 18       | 1                    | 0       | 0    | 0     | 2     | 0    | 0     | 3 | 2.13  | 2.49     | 0.42    | 2.37   |            |
| 19       | 1                    | 0       | 0    | 0     | 2     | 0    | 0     | 3 | 2.18  | 2.41     | 0.3     | 2.38   |            |
| 20       | 1                    | 0       | 0    | 0     | 2     | 0    | 0     | 3 | 2.16  | 2.45     | 0.37    | 2.39   |            |

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

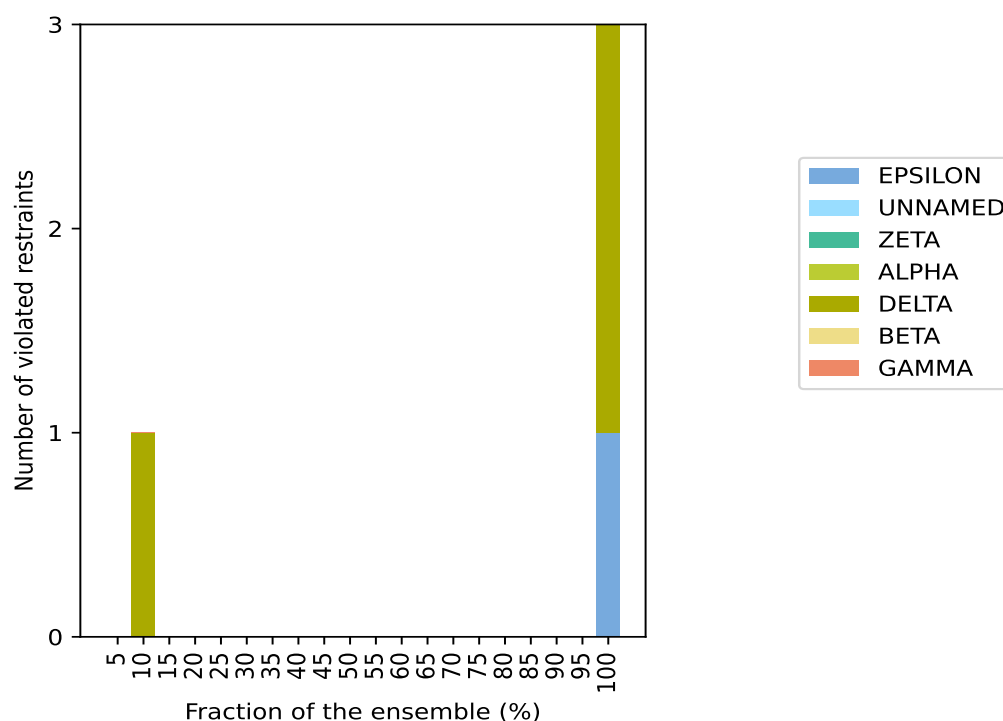
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

| Number of violated restraints |         |      |       |       |      |       |       | Fraction of the ensemble |       |
|-------------------------------|---------|------|-------|-------|------|-------|-------|--------------------------|-------|
| EPSILON                       | UNNAMED | ZETA | ALPHA | DELTA | BETA | GAMMA | Total | Count <sup>1</sup>       | %     |
| 0                             | 0       | 0    | 0     | 0     | 0    | 0     | 0     | 1                        | 5.0   |
| 0                             | 0       | 0    | 0     | 1     | 0    | 0     | 1     | 2                        | 10.0  |
| 0                             | 0       | 0    | 0     | 0     | 0    | 0     | 0     | 3                        | 15.0  |
| 0                             | 0       | 0    | 0     | 0     | 0    | 0     | 0     | 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  |
| 1                             | 0       | 0    | 0     | 2     | 0    | 0     | 3     | 20                       | 100.0 |

<sup>1</sup> Number of models with violations

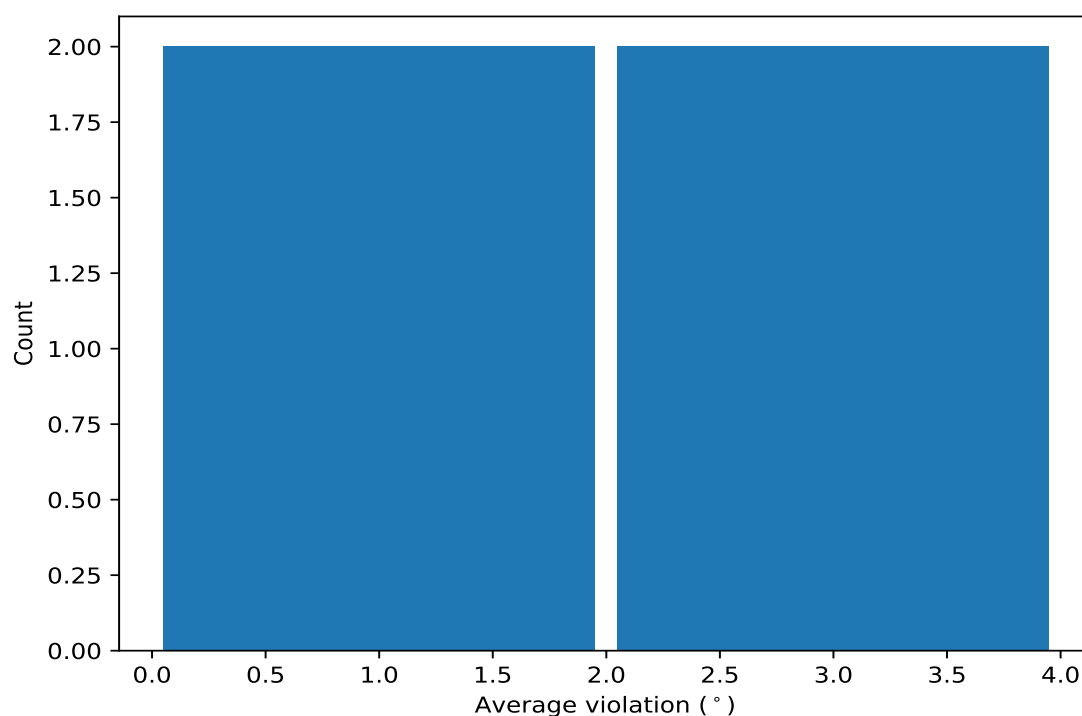
### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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 <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|--------|---------------|---------------|---------------|---------------|---------------------|------|-----------------|--------|
| (1,52) | 1:16:B:DT:C5' | 1:16:B:DT:C4' | 1:16:B:DT:C3' | 1:16:B:DT:O3' | 20                  | 2.44 | 0.1             | 2.43   |
| (1,51) | 1:8:A:DT:C5'  | 1:8:A:DT:C4'  | 1:8:A:DT:C3'  | 1:8:A:DT:O3'  | 20                  | 2.4  | 0.07            | 2.4    |
| (1,58) | 1:12:B:DC:C4' | 1:12:B:DC:C3' | 1:12:B:DC:O3' | 1:13:B:GF2:P  | 20                  | 1.57 | 0.3             | 1.51   |
| (1,45) | 1:4:A:DC:C5'  | 1:4:A:DC:C4'  | 1:4:A:DC:C3'  | 1:4:A:DC:O3'  | 2                   | 1.09 | 0.03            | 1.09   |

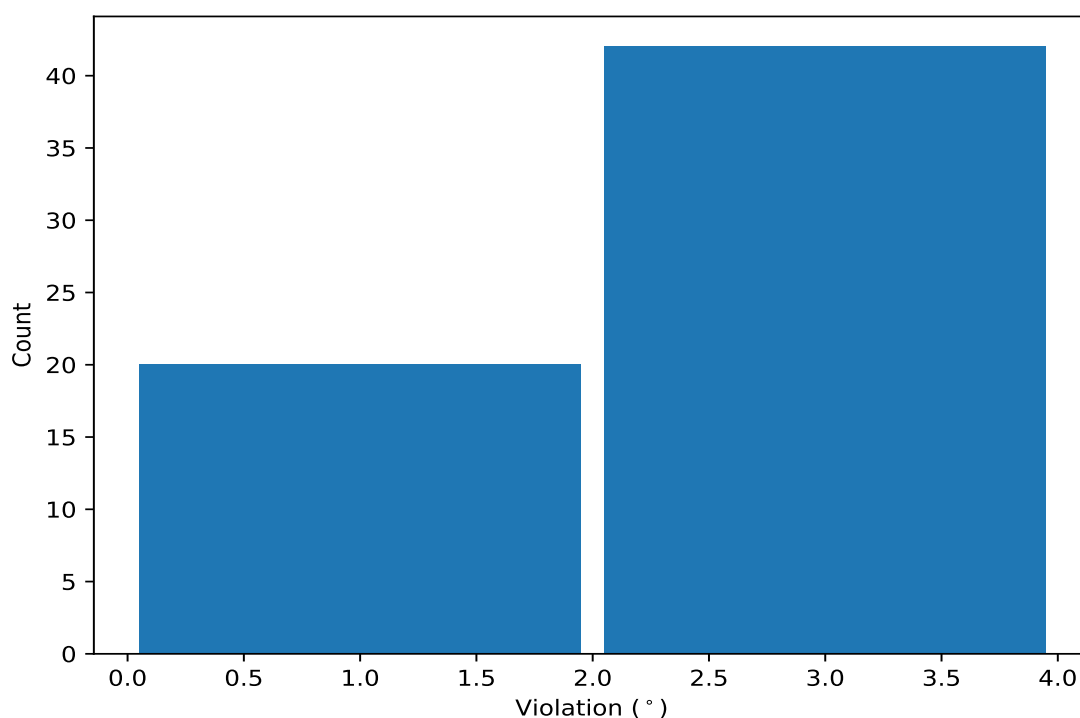
<sup>1</sup> Number of violated models, <sup>2</sup>Standard deviation, All angle values are in degree (°)

### 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 (°) |
|--------|---------------|---------------|---------------|---------------|----------|---------------|
| (1,52) | 1:16:B:DT:C5' | 1:16:B:DT:C4' | 1:16:B:DT:C3' | 1:16:B:DT:O3' | 2        | 2.6           |
| (1,52) | 1:16:B:DT:C5' | 1:16:B:DT:C4' | 1:16:B:DT:C3' | 1:16:B:DT:O3' | 9        | 2.6           |
| (1,52) | 1:16:B:DT:C5' | 1:16:B:DT:C4' | 1:16:B:DT:C3' | 1:16:B:DT:O3' | 4        | 2.54          |
| (1,52) | 1:16:B:DT:C5' | 1:16:B:DT:C4' | 1:16:B:DT:C3' | 1:16:B:DT:O3' | 5        | 2.54          |
| (1,52) | 1:16:B:DT:C5' | 1:16:B:DT:C4' | 1:16:B:DT:C3' | 1:16:B:DT:O3' | 13       | 2.54          |
| (1,52) | 1:16:B:DT:C5' | 1:16:B:DT:C4' | 1:16:B:DT:C3' | 1:16:B:DT:O3' | 17       | 2.53          |
| (1,51) | 1:8:A:DT:C5'  | 1:8:A:DT:C4'  | 1:8:A:DT:C3'  | 1:8:A:DT:O3'  | 14       | 2.53          |
| (1,52) | 1:16:B:DT:C5' | 1:16:B:DT:C4' | 1:16:B:DT:C3' | 1:16:B:DT:O3' | 6        | 2.52          |
| (1,52) | 1:16:B:DT:C5' | 1:16:B:DT:C4' | 1:16:B:DT:C3' | 1:16:B:DT:O3' | 12       | 2.51          |
| (1,51) | 1:8:A:DT:C5'  | 1:8:A:DT:C4'  | 1:8:A:DT:C3'  | 1:8:A:DT:O3'  | 15       | 2.5           |