



## Full wwPDB EM Validation Report ⓘ

Jul 15, 2026 – 04:08 AM JST

PDB ID : 9VWG / pdb\_00009vwg  
EMDB ID : EMD-65396  
Title : Structure of 16-mer V.cholerae dGTPase H114A bound to dGTP and dAMP  
Authors : Shi, M.; Li, P.P.; Li, Q.J.; Gao, A.  
Deposited on : 2025-07-17  
Resolution : 3.29 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

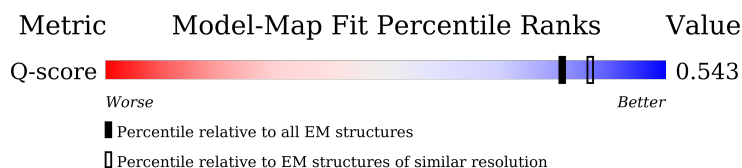
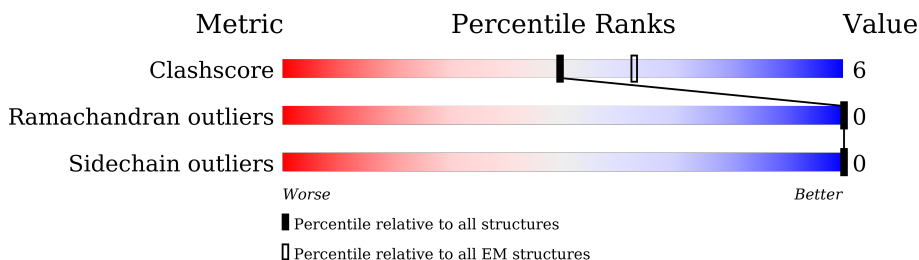
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.29 Å.

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.



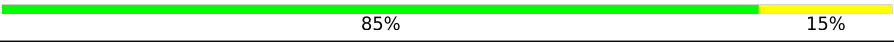
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 14466 ( 2.79 - 3.79 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 402    |                  |
| 1   | B     | 402    |                  |
| 1   | C     | 402    |                  |
| 1   | D     | 402    |                  |

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| Mol | Chain | Length | Quality of chain                                                                    |  |
|-----|-------|--------|-------------------------------------------------------------------------------------|--|
| 1   | E     | 402    |   |  |
| 1   | F     | 402    |   |  |
| 1   | G     | 402    |   |  |
| 1   | H     | 402    |   |  |
| 1   | I     | 402    |   |  |
| 1   | J     | 402    |   |  |
| 1   | K     | 402    |   |  |
| 1   | L     | 402    |   |  |
| 1   | M     | 402    |   |  |
| 1   | N     | 402    |   |  |
| 1   | O     | 402    |   |  |
| 1   | P     | 402    |  |  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 52432 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

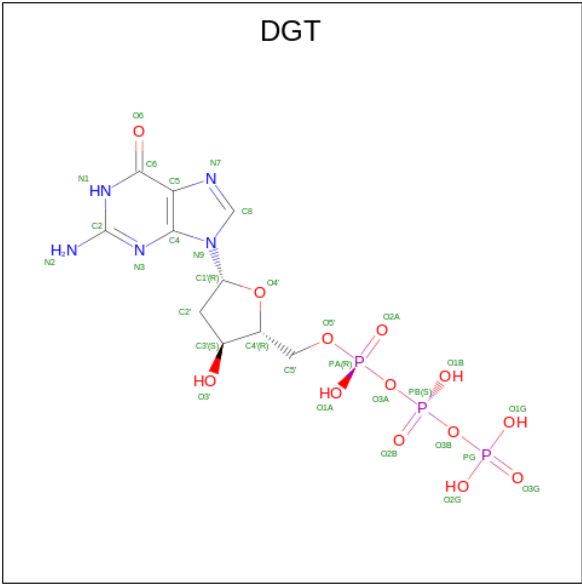
- Molecule 1 is a protein called Deoxyguanosinetriphosphate triphosphohydrolase-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3224  | 2045 | 546 | 617 | 16 |         |       |
| 1   | B     | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3224  | 2045 | 546 | 617 | 16 |         |       |
| 1   | C     | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3224  | 2045 | 546 | 617 | 16 |         |       |
| 1   | D     | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3224  | 2045 | 546 | 617 | 16 |         |       |
| 1   | E     | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3224  | 2045 | 546 | 617 | 16 |         |       |
| 1   | F     | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3224  | 2045 | 546 | 617 | 16 |         |       |
| 1   | G     | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3224  | 2045 | 546 | 617 | 16 |         |       |
| 1   | H     | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3224  | 2045 | 546 | 617 | 16 |         |       |
| 1   | I     | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3224  | 2045 | 546 | 617 | 16 |         |       |
| 1   | J     | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3224  | 2045 | 546 | 617 | 16 |         |       |
| 1   | K     | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3224  | 2045 | 546 | 617 | 16 |         |       |
| 1   | L     | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3224  | 2045 | 546 | 617 | 16 |         |       |
| 1   | M     | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3224  | 2045 | 546 | 617 | 16 |         |       |
| 1   | N     | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3224  | 2045 | 546 | 617 | 16 |         |       |
| 1   | O     | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3224  | 2045 | 546 | 617 | 16 |         |       |
| 1   | P     | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3224  | 2045 | 546 | 617 | 16 |         |       |

There are 16 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference      |
|-------|---------|----------|--------|---------------------|----------------|
| A     | 114     | ALA      | HIS    | engineered mutation | UNP A0A0H6GV99 |
| B     | 114     | ALA      | HIS    | engineered mutation | UNP A0A0H6GV99 |
| C     | 114     | ALA      | HIS    | engineered mutation | UNP A0A0H6GV99 |
| D     | 114     | ALA      | HIS    | engineered mutation | UNP A0A0H6GV99 |
| E     | 114     | ALA      | HIS    | engineered mutation | UNP A0A0H6GV99 |
| F     | 114     | ALA      | HIS    | engineered mutation | UNP A0A0H6GV99 |
| G     | 114     | ALA      | HIS    | engineered mutation | UNP A0A0H6GV99 |
| H     | 114     | ALA      | HIS    | engineered mutation | UNP A0A0H6GV99 |
| I     | 114     | ALA      | HIS    | engineered mutation | UNP A0A0H6GV99 |
| J     | 114     | ALA      | HIS    | engineered mutation | UNP A0A0H6GV99 |
| K     | 114     | ALA      | HIS    | engineered mutation | UNP A0A0H6GV99 |
| L     | 114     | ALA      | HIS    | engineered mutation | UNP A0A0H6GV99 |
| M     | 114     | ALA      | HIS    | engineered mutation | UNP A0A0H6GV99 |
| N     | 114     | ALA      | HIS    | engineered mutation | UNP A0A0H6GV99 |
| O     | 114     | ALA      | HIS    | engineered mutation | UNP A0A0H6GV99 |
| P     | 114     | ALA      | HIS    | engineered mutation | UNP A0A0H6GV99 |

- Molecule 2 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



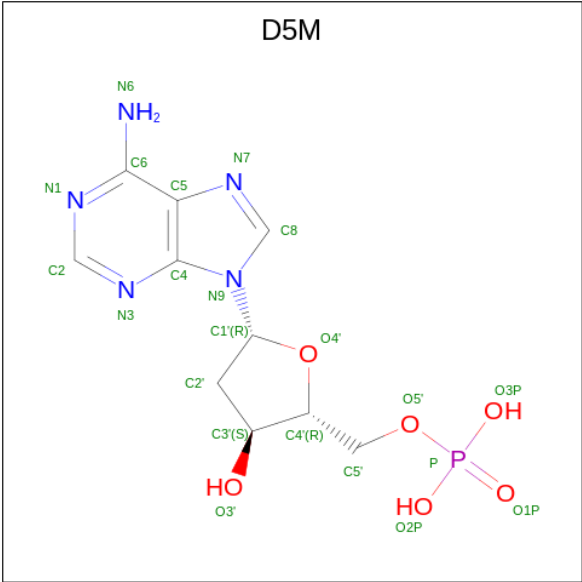
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 2   | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | B     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | C     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 2   | D     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | E     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | F     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | G     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | H     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | I     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | J     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | K     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | L     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | M     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | N     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | O     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | P     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

- Molecule 3 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (CCD ID: D5M) (formula:  $C_{10}H_{14}N_5O_6P$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 3   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |
| 3   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |
| 3   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |
| 3   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |
| 3   | E     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |
| 3   | F     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |
| 3   | G     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |
| 3   | H     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |
| 3   | I     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |
| 3   | J     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |
| 3   | K     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |
| 3   | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |
| 3   | M     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |
| 3   | N     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |

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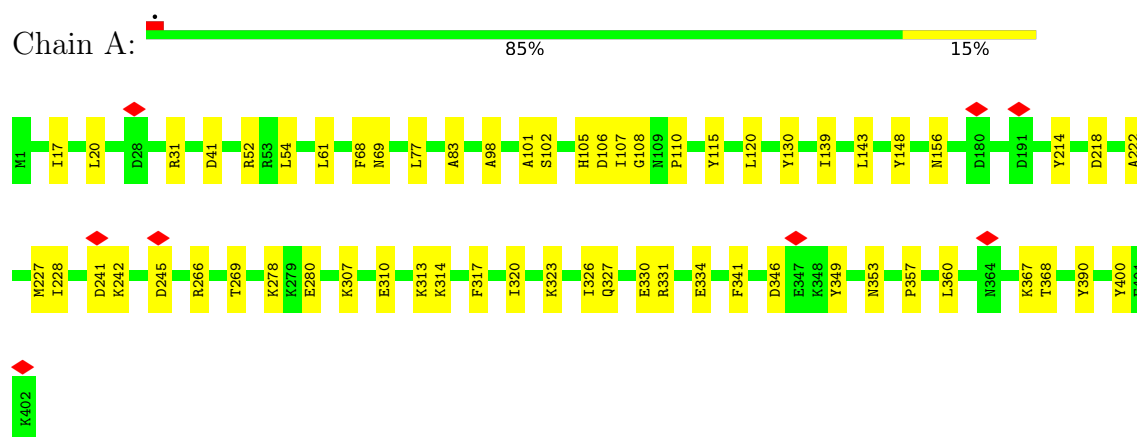
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 3   | O     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |
| 3   | P     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |



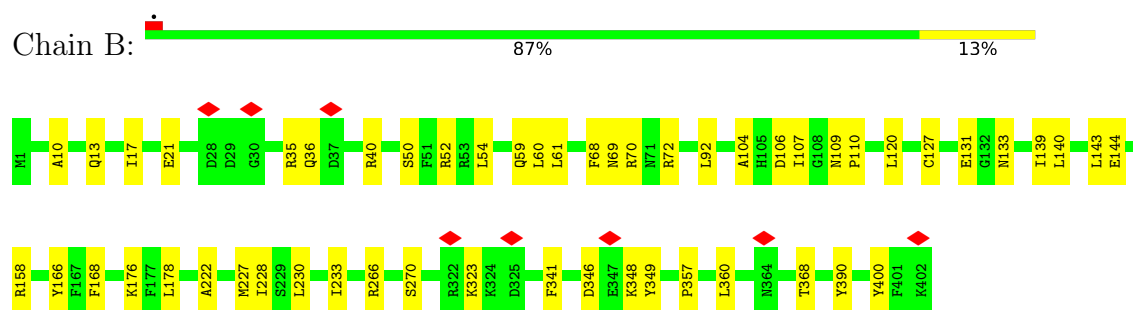
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

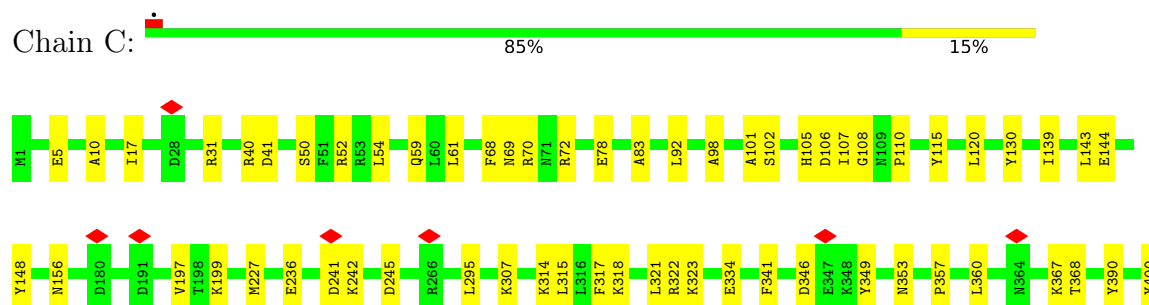
- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein



- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein



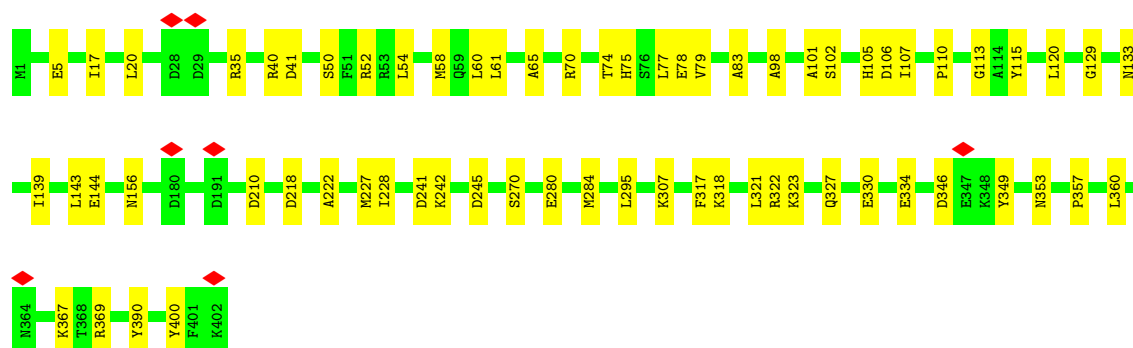
- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein





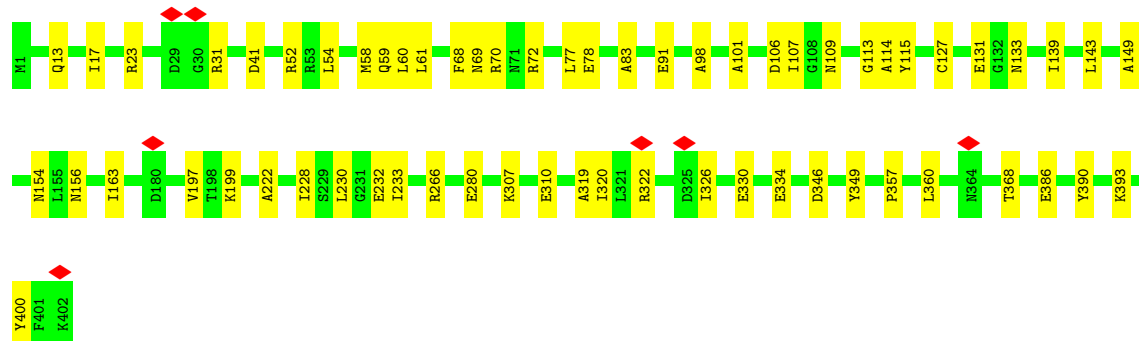
- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein

Chain D: 84% 16%



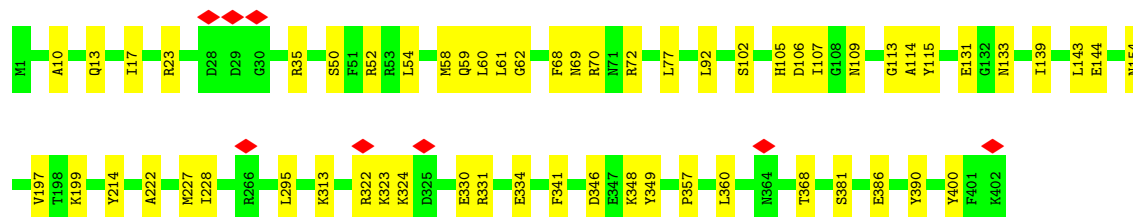
- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein

Chain E: 85% 15%



- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein

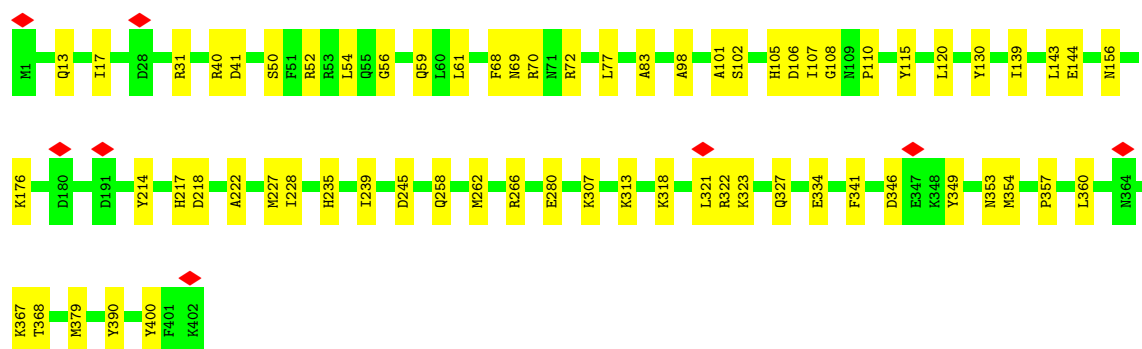
Chain F: 86% 14%



- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein

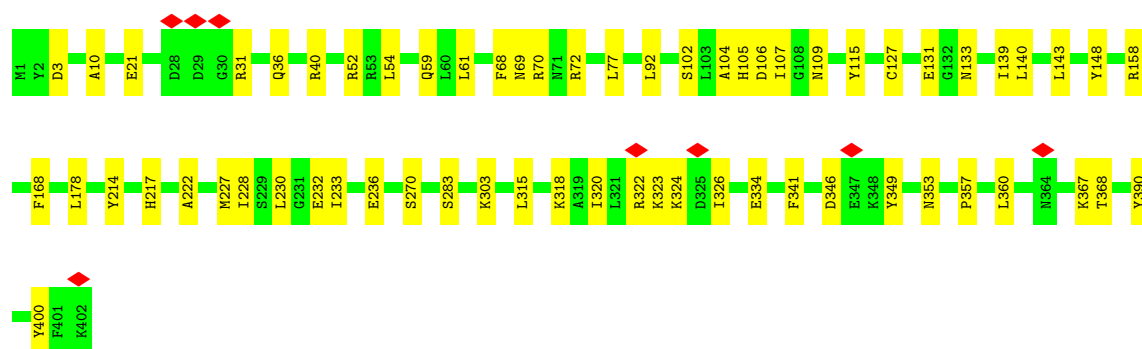
Chain G: 84% 16%





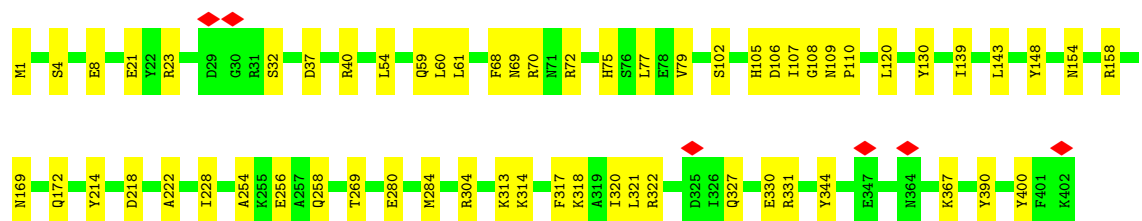
- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein

Chain H: 84% 16%



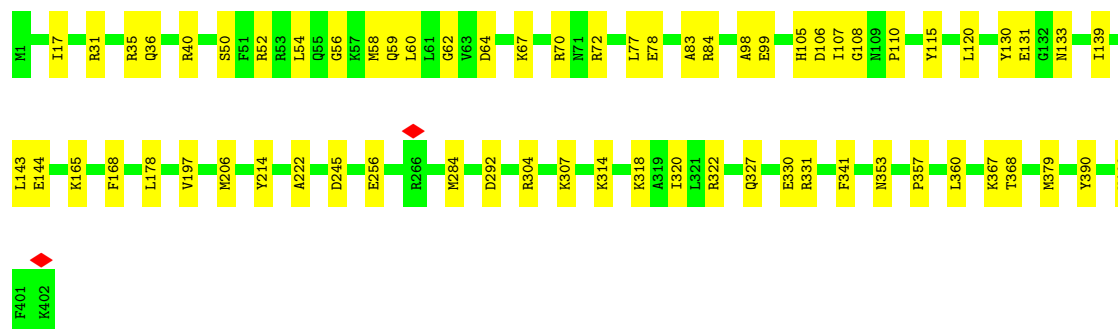
- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein

Chain I: 85% 15%

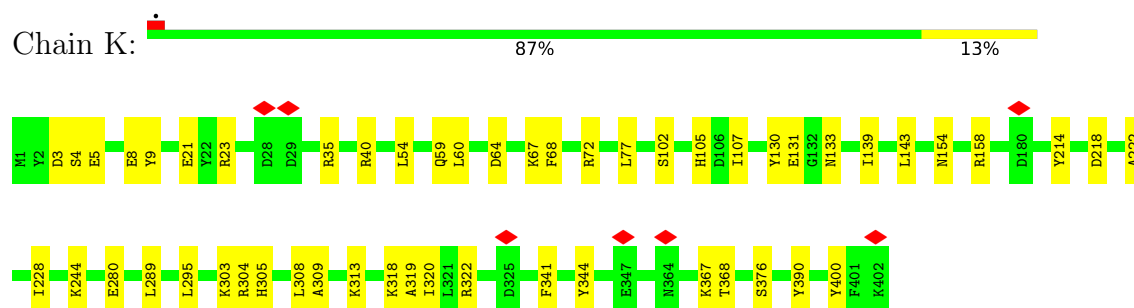


- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein

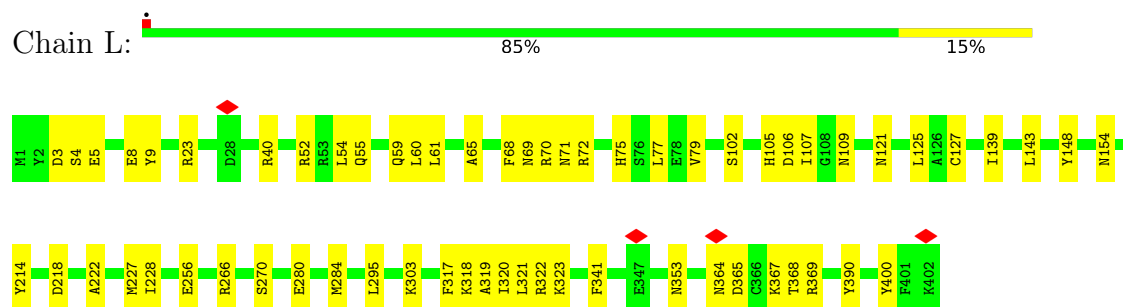
Chain J: 84% 16%



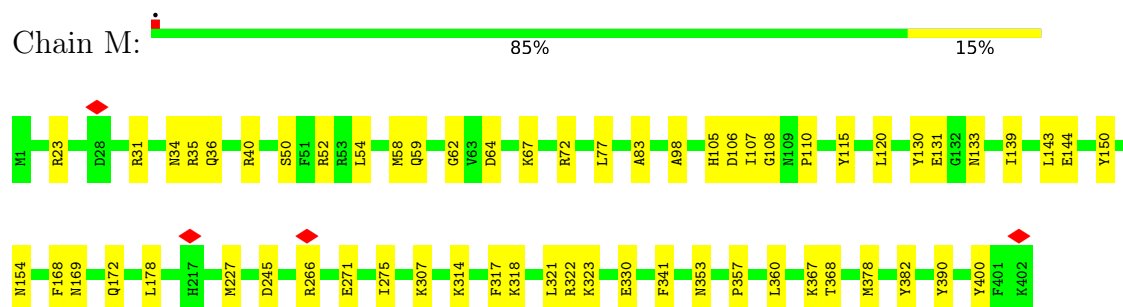
- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein



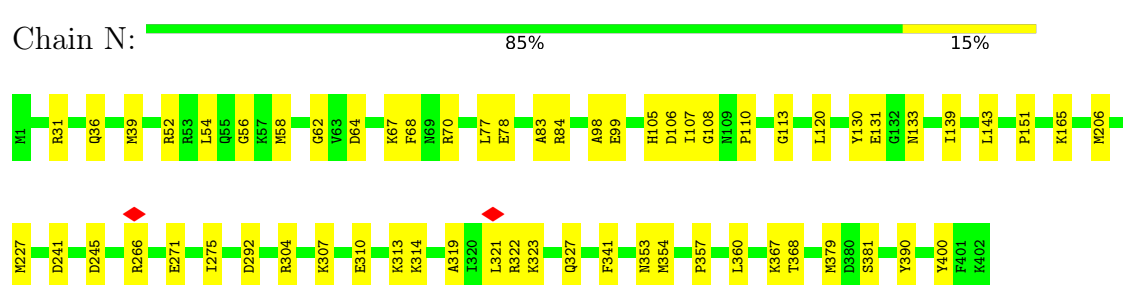
- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein



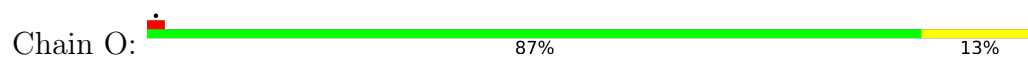
- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein

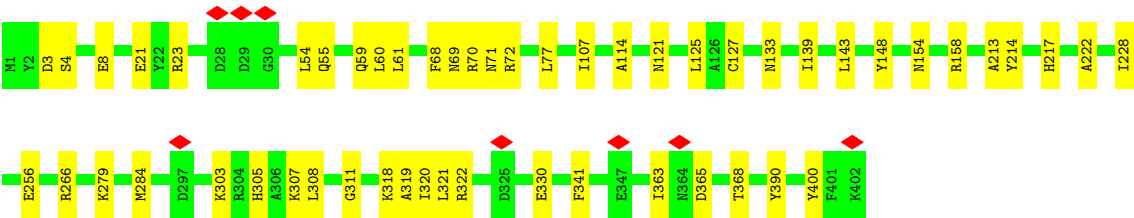


- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein

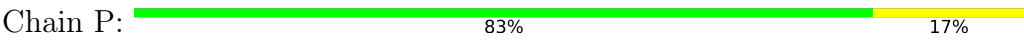


- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein





• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase-like protein



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 51445                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                                      | Depositor |
| Minimum defocus (nm)                 | 1200                                    | Depositor |
| Maximum defocus (nm)                 | 1800                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 3.727                                   | Depositor |
| Minimum map value                    | -2.178                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.153                                   | Depositor |
| Recommended contour level            | 0.6                                     | Depositor |
| Map size ( $\text{\AA}$ )            | 332.8, 332.8, 332.8                     | wwPDB     |
| Map dimensions                       | 320, 320, 320                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.04, 1.04, 1.04                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D5M, DGT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | A     | 0.11         | 0/3279  | 0.25        | 0/4407  |
| 1   | B     | 0.12         | 0/3279  | 0.25        | 0/4407  |
| 1   | C     | 0.11         | 0/3279  | 0.26        | 0/4407  |
| 1   | D     | 0.11         | 0/3279  | 0.24        | 0/4407  |
| 1   | E     | 0.12         | 0/3279  | 0.25        | 0/4407  |
| 1   | F     | 0.12         | 0/3279  | 0.26        | 0/4407  |
| 1   | G     | 0.11         | 0/3279  | 0.25        | 0/4407  |
| 1   | H     | 0.11         | 0/3279  | 0.25        | 0/4407  |
| 1   | I     | 0.12         | 0/3279  | 0.29        | 0/4407  |
| 1   | J     | 0.12         | 0/3279  | 0.25        | 0/4407  |
| 1   | K     | 0.16         | 0/3279  | 0.29        | 0/4407  |
| 1   | L     | 0.12         | 0/3279  | 0.29        | 0/4407  |
| 1   | M     | 0.19         | 0/3279  | 0.31        | 0/4407  |
| 1   | N     | 0.12         | 0/3279  | 0.25        | 0/4407  |
| 1   | O     | 0.20         | 0/3279  | 0.30        | 0/4407  |
| 1   | P     | 0.12         | 0/3279  | 0.25        | 0/4407  |
| All | All   | 0.13         | 0/52464 | 0.27        | 0/70512 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3224  | 0        | 3218     | 40      | 0            |
| 1   | B     | 3224  | 0        | 3218     | 33      | 0            |
| 1   | C     | 3224  | 0        | 3218     | 38      | 0            |
| 1   | D     | 3224  | 0        | 3218     | 45      | 0            |
| 1   | E     | 3224  | 0        | 3218     | 43      | 0            |
| 1   | F     | 3224  | 0        | 3218     | 40      | 0            |
| 1   | G     | 3224  | 0        | 3218     | 46      | 0            |
| 1   | H     | 3224  | 0        | 3218     | 41      | 0            |
| 1   | I     | 3224  | 0        | 3218     | 40      | 0            |
| 1   | J     | 3224  | 0        | 3218     | 41      | 0            |
| 1   | K     | 3224  | 0        | 3218     | 33      | 0            |
| 1   | L     | 3224  | 0        | 3218     | 48      | 0            |
| 1   | M     | 3224  | 0        | 3218     | 41      | 0            |
| 1   | N     | 3224  | 0        | 3218     | 42      | 0            |
| 1   | O     | 3224  | 0        | 3218     | 38      | 0            |
| 1   | P     | 3224  | 0        | 3218     | 48      | 0            |
| 2   | A     | 31    | 0        | 12       | 2       | 0            |
| 2   | B     | 31    | 0        | 12       | 1       | 0            |
| 2   | C     | 31    | 0        | 12       | 0       | 0            |
| 2   | D     | 31    | 0        | 12       | 3       | 0            |
| 2   | E     | 31    | 0        | 12       | 2       | 0            |
| 2   | F     | 31    | 0        | 12       | 2       | 0            |
| 2   | G     | 31    | 0        | 12       | 3       | 0            |
| 2   | H     | 31    | 0        | 12       | 0       | 0            |
| 2   | I     | 31    | 0        | 12       | 2       | 0            |
| 2   | J     | 31    | 0        | 12       | 3       | 0            |
| 2   | K     | 31    | 0        | 12       | 1       | 0            |
| 2   | L     | 31    | 0        | 12       | 2       | 0            |
| 2   | M     | 31    | 0        | 12       | 0       | 0            |
| 2   | N     | 31    | 0        | 12       | 0       | 0            |
| 2   | O     | 31    | 0        | 12       | 6       | 0            |
| 2   | P     | 31    | 0        | 12       | 2       | 0            |
| 3   | A     | 22    | 0        | 12       | 1       | 0            |
| 3   | B     | 22    | 0        | 12       | 1       | 0            |
| 3   | C     | 22    | 0        | 12       | 2       | 0            |
| 3   | D     | 22    | 0        | 12       | 2       | 0            |
| 3   | E     | 22    | 0        | 12       | 1       | 0            |
| 3   | F     | 22    | 0        | 12       | 1       | 0            |
| 3   | G     | 22    | 0        | 12       | 2       | 0            |
| 3   | H     | 22    | 0        | 12       | 0       | 0            |
| 3   | I     | 22    | 0        | 12       | 0       | 0            |
| 3   | J     | 22    | 0        | 12       | 1       | 0            |
| 3   | K     | 22    | 0        | 12       | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | L     | 22    | 0        | 12       | 1       | 0            |
| 3   | M     | 22    | 0        | 12       | 1       | 0            |
| 3   | N     | 22    | 0        | 12       | 1       | 0            |
| 3   | O     | 22    | 0        | 12       | 0       | 0            |
| 3   | P     | 22    | 0        | 12       | 2       | 0            |
| All | All   | 52432 | 0        | 51872    | 596     | 0            |

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 6.

All (596) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:115:TYR:HB3  | 1:M:330:GLU:OE1  | 1.69                     | 0.92              |
| 1:C:236:GLU:HB3  | 1:C:315:LEU:HD12 | 1.58                     | 0.82              |
| 1:M:115:TYR:CB   | 1:M:330:GLU:OE1  | 2.29                     | 0.80              |
| 1:F:139:ILE:HG12 | 1:F:143:LEU:HD12 | 1.68                     | 0.76              |
| 1:H:139:ILE:HG12 | 1:H:143:LEU:HD12 | 1.67                     | 0.74              |
| 1:B:59:GLN:OE1   | 1:B:72:ARG:NH1   | 2.23                     | 0.72              |
| 1:F:114:ALA:HB3  | 2:F:501:DGT:C5   | 2.19                     | 0.72              |
| 1:P:139:ILE:HA   | 1:P:143:LEU:HB2  | 1.71                     | 0.72              |
| 1:H:318:LYS:HE2  | 1:H:322:ARG:HH21 | 1.54                     | 0.72              |
| 1:J:115:TYR:HD1  | 1:J:330:GLU:HB3  | 1.56                     | 0.71              |
| 1:E:59:GLN:OE1   | 1:E:72:ARG:NH1   | 2.24                     | 0.71              |
| 1:L:106:ASP:OD1  | 1:L:109:ASN:ND2  | 2.22                     | 0.71              |
| 1:K:59:GLN:OE1   | 1:K:72:ARG:NH1   | 2.25                     | 0.70              |
| 1:E:139:ILE:HG12 | 1:E:143:LEU:HD12 | 1.73                     | 0.70              |
| 1:B:68:PHE:O     | 1:C:52:ARG:NH1   | 2.25                     | 0.70              |
| 1:C:59:GLN:OE1   | 1:C:72:ARG:NH1   | 2.24                     | 0.70              |
| 1:A:54:LEU:HD21  | 1:A:107:ILE:HA   | 1.74                     | 0.69              |
| 1:D:54:LEU:HD21  | 1:D:107:ILE:HA   | 1.74                     | 0.69              |
| 1:B:166:TYR:CD2  | 1:B:176:LYS:HB3  | 2.27                     | 0.69              |
| 1:G:54:LEU:HD21  | 1:G:107:ILE:HA   | 1.73                     | 0.69              |
| 1:C:54:LEU:HD21  | 1:C:107:ILE:HA   | 1.73                     | 0.69              |
| 1:H:54:LEU:HD21  | 1:H:107:ILE:HA   | 1.75                     | 0.69              |
| 1:D:280:GLU:HG3  | 1:D:284:MET:HE3  | 1.73                     | 0.68              |
| 1:B:52:ARG:NH1   | 1:C:68:PHE:O     | 2.27                     | 0.68              |
| 1:I:54:LEU:HD21  | 1:I:107:ILE:HA   | 1.75                     | 0.68              |
| 1:O:59:GLN:OE1   | 1:O:72:ARG:NH1   | 2.26                     | 0.67              |
| 1:H:59:GLN:OE1   | 1:H:72:ARG:NH1   | 2.27                     | 0.67              |
| 1:B:139:ILE:HG12 | 1:B:143:LEU:HD12 | 1.76                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:59:GLN:OE1   | 1:I:72:ARG:NH1   | 2.28                     | 0.66              |
| 1:A:52:ARG:NH1   | 1:E:68:PHE:O     | 2.28                     | 0.66              |
| 1:D:52:ARG:NH1   | 1:F:68:PHE:O     | 2.27                     | 0.66              |
| 1:J:139:ILE:HG12 | 1:J:143:LEU:HD12 | 1.78                     | 0.66              |
| 1:L:59:GLN:OE1   | 1:L:72:ARG:NH1   | 2.29                     | 0.66              |
| 1:L:54:LEU:HD21  | 1:L:107:ILE:HA   | 1.77                     | 0.66              |
| 1:L:318:LYS:HE2  | 1:L:322:ARG:HH21 | 1.59                     | 0.66              |
| 1:G:139:ILE:HG12 | 1:G:143:LEU:HD12 | 1.77                     | 0.66              |
| 1:E:54:LEU:HD21  | 1:E:107:ILE:HA   | 1.79                     | 0.65              |
| 1:M:390:TYR:HB3  | 1:N:400:TYR:HB2  | 1.79                     | 0.65              |
| 1:G:52:ARG:NH1   | 1:H:68:PHE:O     | 2.30                     | 0.65              |
| 1:L:68:PHE:O     | 1:N:52:ARG:NH1   | 2.30                     | 0.65              |
| 1:N:58:MET:HG3   | 1:N:62:GLY:HA2   | 1.79                     | 0.65              |
| 1:O:54:LEU:HD21  | 1:O:107:ILE:HA   | 1.78                     | 0.65              |
| 1:B:54:LEU:HD21  | 1:B:107:ILE:HA   | 1.80                     | 0.64              |
| 1:D:322:ARG:HH12 | 1:H:270:SER:H    | 1.45                     | 0.64              |
| 1:N:354:MET:HB3  | 1:P:327:GLN:NE2  | 2.13                     | 0.64              |
| 1:K:54:LEU:HD21  | 1:K:107:ILE:HA   | 1.79                     | 0.63              |
| 1:F:54:LEU:HD21  | 1:F:107:ILE:HA   | 1.80                     | 0.63              |
| 1:M:54:LEU:HD21  | 1:M:107:ILE:HA   | 1.80                     | 0.63              |
| 1:P:320:ILE:HG22 | 1:P:326:ILE:HG13 | 1.80                     | 0.63              |
| 1:I:318:LYS:O    | 1:I:322:ARG:HG3  | 1.99                     | 0.63              |
| 1:L:148:TYR:O    | 1:N:266:ARG:NH1  | 2.32                     | 0.63              |
| 1:O:68:PHE:O     | 1:P:52:ARG:NH1   | 2.31                     | 0.63              |
| 1:P:54:LEU:HD21  | 1:P:107:ILE:HA   | 1.81                     | 0.63              |
| 1:K:214:TYR:HE1  | 1:K:313:LYS:HG3  | 1.64                     | 0.62              |
| 1:G:214:TYR:HE2  | 1:G:313:LYS:HG2  | 1.64                     | 0.62              |
| 1:O:139:ILE:HG12 | 1:O:143:LEU:HD12 | 1.80                     | 0.62              |
| 1:J:54:LEU:HD21  | 1:J:107:ILE:HA   | 1.81                     | 0.62              |
| 1:J:390:TYR:HB3  | 1:M:400:TYR:HB2  | 1.82                     | 0.62              |
| 1:O:319:ALA:HA   | 1:O:322:ARG:HE   | 1.64                     | 0.62              |
| 1:I:23:ARG:NH1   | 1:I:154:ASN:O    | 2.30                     | 0.62              |
| 1:I:68:PHE:O     | 1:M:52:ARG:NH1   | 2.33                     | 0.62              |
| 1:J:400:TYR:HB2  | 1:P:390:TYR:HB3  | 1.82                     | 0.61              |
| 1:G:59:GLN:OE1   | 1:G:72:ARG:NH1   | 2.33                     | 0.61              |
| 1:O:148:TYR:O    | 1:P:266:ARG:NH1  | 2.34                     | 0.61              |
| 1:N:390:TYR:HB3  | 1:P:400:TYR:HB2  | 1.83                     | 0.61              |
| 1:D:35:ARG:HE    | 1:D:40:ARG:HG2   | 1.66                     | 0.61              |
| 1:G:68:PHE:O     | 1:H:52:ARG:NH1   | 2.33                     | 0.60              |
| 1:K:5:GLU:HG2    | 1:K:295:LEU:HD12 | 1.82                     | 0.60              |
| 1:N:54:LEU:HD21  | 1:N:107:ILE:HA   | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:313:LYS:HE3  | 1:N:314:LYS:HE3  | 1.83                     | 0.60              |
| 1:A:68:PHE:O     | 1:E:52:ARG:NH1   | 2.34                     | 0.60              |
| 1:K:390:TYR:HB3  | 1:O:400:TYR:HB2  | 1.84                     | 0.60              |
| 1:P:310:GLU:OE2  | 1:P:314:LYS:NZ   | 2.28                     | 0.60              |
| 1:B:61:LEU:HB2   | 1:B:69:ASN:HD21  | 1.67                     | 0.59              |
| 1:M:317:PHE:HD2  | 1:M:321:LEU:HD13 | 1.67                     | 0.59              |
| 1:J:70:ARG:NE    | 1:J:78:GLU:OE2   | 2.35                     | 0.59              |
| 1:M:139:ILE:HG12 | 1:M:143:LEU:HD12 | 1.83                     | 0.59              |
| 1:A:390:TYR:HB3  | 1:C:400:TYR:HB2  | 1.84                     | 0.59              |
| 1:I:390:TYR:HB3  | 1:K:400:TYR:HB2  | 1.85                     | 0.58              |
| 1:A:41:ASP:OD2   | 1:A:156:ASN:ND2  | 2.29                     | 0.58              |
| 1:E:390:TYR:HB3  | 1:F:400:TYR:HB2  | 1.85                     | 0.58              |
| 1:H:222:ALA:HB1  | 1:H:228:ILE:HG22 | 1.86                     | 0.58              |
| 1:C:31:ARG:NH1   | 3:C:502:D5M:O1P  | 2.34                     | 0.58              |
| 1:E:131:GLU:HG2  | 1:E:133:ASN:H    | 1.69                     | 0.58              |
| 1:G:70:ARG:HG3   | 1:G:217:HIS:HD2  | 1.69                     | 0.58              |
| 1:E:222:ALA:HB1  | 1:E:228:ILE:HG22 | 1.85                     | 0.58              |
| 1:O:114:ALA:HB3  | 2:O:501:DGT:N7   | 2.18                     | 0.58              |
| 1:H:236:GLU:HB3  | 1:H:315:LEU:HD23 | 1.85                     | 0.57              |
| 1:C:5:GLU:HG2    | 1:C:295:LEU:HD12 | 1.85                     | 0.57              |
| 1:D:357:PRO:HD2  | 1:D:360:LEU:HD12 | 1.86                     | 0.57              |
| 1:C:357:PRO:HD2  | 1:C:360:LEU:HD12 | 1.87                     | 0.57              |
| 1:C:318:LYS:HE2  | 1:C:322:ARG:HH21 | 1.68                     | 0.57              |
| 1:D:139:ILE:HG12 | 1:D:143:LEU:HD12 | 1.87                     | 0.57              |
| 1:I:400:TYR:HB2  | 1:L:390:TYR:HB3  | 1.87                     | 0.57              |
| 1:F:357:PRO:HD2  | 1:F:360:LEU:HD12 | 1.87                     | 0.57              |
| 1:O:77:LEU:HD11  | 1:P:77:LEU:HD11  | 1.87                     | 0.57              |
| 1:F:131:GLU:HG2  | 1:F:133:ASN:H    | 1.70                     | 0.57              |
| 1:H:131:GLU:HG2  | 1:H:133:ASN:H    | 1.70                     | 0.57              |
| 1:B:106:ASP:OD1  | 1:B:109:ASN:ND2  | 2.38                     | 0.56              |
| 1:C:390:TYR:HB3  | 1:G:400:TYR:HB2  | 1.87                     | 0.56              |
| 1:E:357:PRO:HD2  | 1:E:360:LEU:HD12 | 1.86                     | 0.56              |
| 1:L:400:TYR:HB2  | 1:O:390:TYR:HB3  | 1.87                     | 0.56              |
| 1:D:245:ASP:HB3  | 1:D:307:LYS:HD3  | 1.87                     | 0.56              |
| 1:L:5:GLU:HG2    | 1:L:295:LEU:HD12 | 1.86                     | 0.56              |
| 1:N:227:MET:HE2  | 1:N:323:LYS:HG3  | 1.86                     | 0.56              |
| 1:A:400:TYR:HB2  | 1:D:390:TYR:HB3  | 1.88                     | 0.56              |
| 1:B:357:PRO:HD2  | 1:B:360:LEU:HD12 | 1.87                     | 0.56              |
| 1:H:61:LEU:HB2   | 1:H:69:ASN:HD21  | 1.71                     | 0.56              |
| 1:B:390:TYR:HB3  | 1:E:400:TYR:HB2  | 1.88                     | 0.56              |
| 1:A:357:PRO:HD2  | 1:A:360:LEU:HD12 | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:106:ASP:OD1  | 1:F:109:ASN:ND2  | 2.39                     | 0.56              |
| 1:L:106:ASP:HA   | 1:L:109:ASN:ND2  | 2.20                     | 0.56              |
| 1:G:357:PRO:HD2  | 1:G:360:LEU:HD12 | 1.88                     | 0.56              |
| 1:F:61:LEU:HB2   | 1:F:69:ASN:HD21  | 1.70                     | 0.56              |
| 1:J:318:LYS:O    | 1:J:322:ARG:HG3  | 2.05                     | 0.56              |
| 1:K:318:LYS:HE2  | 1:K:322:ARG:HH21 | 1.71                     | 0.56              |
| 1:M:58:MET:HG3   | 1:M:62:GLY:HA2   | 1.88                     | 0.56              |
| 1:F:390:TYR:HB3  | 1:H:400:TYR:HB2  | 1.88                     | 0.55              |
| 1:M:318:LYS:O    | 1:M:322:ARG:HG3  | 2.06                     | 0.55              |
| 1:C:139:ILE:HG12 | 1:C:143:LEU:HD12 | 1.88                     | 0.55              |
| 1:F:330:GLU:OE2  | 2:F:501:DGT:N1   | 2.36                     | 0.55              |
| 1:B:69:ASN:OD1   | 1:B:70:ARG:N     | 2.40                     | 0.55              |
| 1:M:50:SER:OG    | 1:M:144:GLU:OE2  | 2.20                     | 0.55              |
| 1:A:139:ILE:HG12 | 1:A:143:LEU:HD12 | 1.88                     | 0.55              |
| 1:D:400:TYR:HB2  | 1:G:390:TYR:HB3  | 1.88                     | 0.55              |
| 1:L:65:ALA:O     | 1:N:381:SER:OG   | 2.23                     | 0.55              |
| 1:H:357:PRO:HD2  | 1:H:360:LEU:HD12 | 1.87                     | 0.55              |
| 1:I:148:TYR:O    | 1:M:266:ARG:NH1  | 2.40                     | 0.55              |
| 1:B:266:ARG:NH1  | 1:C:148:TYR:O    | 2.39                     | 0.55              |
| 1:F:69:ASN:OD1   | 1:F:70:ARG:N     | 2.39                     | 0.55              |
| 1:M:59:GLN:OE1   | 1:M:72:ARG:NH1   | 2.39                     | 0.55              |
| 1:P:59:GLN:OE1   | 1:P:72:ARG:NH1   | 2.40                     | 0.55              |
| 1:B:400:TYR:HB2  | 1:H:390:TYR:HB3  | 1.89                     | 0.55              |
| 1:H:106:ASP:OD1  | 1:H:109:ASN:ND2  | 2.39                     | 0.54              |
| 1:J:60:LEU:HD12  | 2:J:501:DGT:H2'  | 1.89                     | 0.54              |
| 1:N:56:GLY:HA3   | 1:N:379:MET:HE2  | 1.88                     | 0.54              |
| 1:E:69:ASN:OD1   | 1:E:70:ARG:N     | 2.39                     | 0.54              |
| 1:F:23:ARG:NH1   | 1:F:154:ASN:O    | 2.39                     | 0.54              |
| 1:H:69:ASN:OD1   | 1:H:70:ARG:N     | 2.40                     | 0.54              |
| 1:I:77:LEU:HD11  | 1:M:77:LEU:HD11  | 1.89                     | 0.54              |
| 1:J:35:ARG:HH21  | 1:J:40:ARG:HG2   | 1.71                     | 0.54              |
| 1:K:3:ASP:OD2    | 1:K:303:LYS:NZ   | 2.31                     | 0.54              |
| 1:K:130:TYR:OH   | 1:K:376:SER:HB2  | 2.06                     | 0.54              |
| 1:D:5:GLU:HG2    | 1:D:295:LEU:HD12 | 1.90                     | 0.54              |
| 1:G:218:ASP:OD2  | 2:G:501:DGT:O3'  | 2.26                     | 0.54              |
| 1:O:69:ASN:OD1   | 1:O:70:ARG:N     | 2.41                     | 0.54              |
| 1:A:266:ARG:NH1  | 1:E:149:ALA:O    | 2.40                     | 0.54              |
| 1:L:77:LEU:HD11  | 1:N:77:LEU:HD11  | 1.90                     | 0.54              |
| 1:E:61:LEU:HB2   | 1:E:69:ASN:HD21  | 1.73                     | 0.54              |
| 1:E:106:ASP:OD1  | 1:E:109:ASN:ND2  | 2.40                     | 0.54              |
| 1:L:318:LYS:O    | 1:L:322:ARG:HG3  | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:256:GLU:HB3  | 1:J:284:MET:HE1  | 1.89                     | 0.53              |
| 1:J:327:GLN:NE2  | 1:P:354:MET:HB3  | 2.23                     | 0.53              |
| 1:K:40:ARG:NH2   | 3:K:502:D5M:O3P  | 2.38                     | 0.53              |
| 1:A:341:PHE:HZ   | 1:A:368:THR:HG23 | 1.73                     | 0.53              |
| 1:A:353:ASN:OD1  | 1:A:367:LYS:NZ   | 2.40                     | 0.53              |
| 1:F:386:GLU:OE2  | 1:H:324:LYS:NZ   | 2.28                     | 0.53              |
| 1:O:21:GLU:OE2   | 1:O:158:ARG:NH1  | 2.41                     | 0.53              |
| 1:O:266:ARG:NH2  | 1:P:149:ALA:O    | 2.42                     | 0.53              |
| 1:K:60:LEU:HD21  | 1:K:320:ILE:HD12 | 1.91                     | 0.53              |
| 1:L:256:GLU:HB2  | 1:L:284:MET:HE1  | 1.90                     | 0.53              |
| 1:J:58:MET:HG3   | 1:J:62:GLY:HA2   | 1.91                     | 0.53              |
| 1:H:3:ASP:OD2    | 1:H:303:LYS:NZ   | 2.38                     | 0.52              |
| 1:B:222:ALA:HB1  | 1:B:228:ILE:HG22 | 1.91                     | 0.52              |
| 1:E:230:LEU:HD12 | 1:E:233:ILE:HD11 | 1.91                     | 0.52              |
| 1:J:52:ARG:NH1   | 1:K:68:PHE:O     | 2.42                     | 0.52              |
| 1:J:50:SER:OG    | 1:J:144:GLU:OE2  | 2.21                     | 0.52              |
| 1:O:363:ILE:HG22 | 1:O:365:ASP:H    | 1.73                     | 0.52              |
| 1:L:106:ASP:CB   | 1:L:109:ASN:ND2  | 2.73                     | 0.52              |
| 1:N:310:GLU:HA   | 1:N:313:LYS:HE2  | 1.91                     | 0.52              |
| 1:L:317:PHE:HD2  | 1:L:321:LEU:HD13 | 1.75                     | 0.52              |
| 1:C:353:ASN:OD1  | 1:C:367:LYS:NZ   | 2.42                     | 0.52              |
| 1:I:21:GLU:OE2   | 1:I:158:ARG:NH1  | 2.42                     | 0.52              |
| 1:L:69:ASN:OD1   | 1:L:70:ARG:N     | 2.42                     | 0.52              |
| 1:L:280:GLU:OE2  | 1:N:31:ARG:NH1   | 2.43                     | 0.52              |
| 1:P:218:ASP:OD2  | 2:P:501:DGT:O3'  | 2.21                     | 0.52              |
| 1:P:318:LYS:HE2  | 1:P:322:ARG:HH21 | 1.75                     | 0.52              |
| 1:C:41:ASP:OD2   | 1:C:156:ASN:ND2  | 2.30                     | 0.52              |
| 1:J:77:LEU:HD11  | 1:K:77:LEU:HD11  | 1.92                     | 0.52              |
| 1:C:241:ASP:OD1  | 1:C:242:LYS:N    | 2.44                     | 0.51              |
| 1:L:270:SER:H    | 1:P:322:ARG:HH12 | 1.58                     | 0.51              |
| 1:N:321:LEU:CD1  | 1:N:327:GLN:HE22 | 2.23                     | 0.51              |
| 1:I:280:GLU:OE2  | 1:M:31:ARG:NH1   | 2.41                     | 0.51              |
| 1:O:321:LEU:HD21 | 2:O:501:DGT:C2   | 2.40                     | 0.51              |
| 1:P:245:ASP:HB2  | 1:P:307:LYS:HD3  | 1.91                     | 0.51              |
| 1:C:17:ILE:HD11  | 1:C:197:VAL:HG11 | 1.91                     | 0.51              |
| 1:O:60:LEU:HD21  | 1:O:320:ILE:HD12 | 1.93                     | 0.51              |
| 1:O:266:ARG:HG3  | 1:O:266:ARG:HH11 | 1.76                     | 0.51              |
| 1:G:227:MET:HE2  | 1:G:323:LYS:HG3  | 1.92                     | 0.51              |
| 1:I:108:GLY:O    | 1:I:130:TYR:OH   | 2.28                     | 0.51              |
| 1:C:227:MET:HE2  | 1:C:323:LYS:HG3  | 1.93                     | 0.51              |
| 1:F:222:ALA:HB1  | 1:F:228:ILE:HG22 | 1.92                     | 0.51              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:115:TYR:HE2 | 1:H:334:GLU:HB2  | 1.76                     | 0.51              |
| 1:I:61:LEU:HB2  | 1:I:69:ASN:HD21  | 1.75                     | 0.51              |
| 1:N:353:ASN:OD1 | 1:N:367:LYS:NZ   | 2.44                     | 0.51              |
| 1:G:61:LEU:HD12 | 1:G:69:ASN:HD21  | 1.75                     | 0.50              |
| 1:I:69:ASN:OD1  | 1:I:70:ARG:N     | 2.43                     | 0.50              |
| 1:J:245:ASP:HB2 | 1:J:307:LYS:HD3  | 1.93                     | 0.50              |
| 1:M:318:LYS:NZ  | 1:M:322:ARG:HH21 | 2.09                     | 0.50              |
| 1:E:386:GLU:OE2 | 1:F:324:LYS:NZ   | 2.35                     | 0.50              |
| 1:G:353:ASN:OD1 | 1:G:367:LYS:NZ   | 2.42                     | 0.50              |
| 1:N:84:ARG:NH2  | 1:N:99:GLU:OE2   | 2.43                     | 0.50              |
| 1:B:35:ARG:HH21 | 1:B:40:ARG:HG2   | 1.77                     | 0.50              |
| 1:K:21:GLU:OE2  | 1:K:158:ARG:NH1  | 2.42                     | 0.50              |
| 1:L:106:ASP:CA  | 1:L:109:ASN:ND2  | 2.74                     | 0.50              |
| 1:B:131:GLU:HG2 | 1:B:133:ASN:H    | 1.76                     | 0.50              |
| 1:B:346:ASP:HB3 | 1:B:349:TYR:HB3  | 1.93                     | 0.50              |
| 1:M:318:LYS:HZ2 | 1:M:322:ARG:HH21 | 1.60                     | 0.50              |
| 1:N:319:ALA:HA  | 1:N:322:ARG:HH11 | 1.76                     | 0.50              |
| 1:J:59:GLN:OE1  | 1:J:72:ARG:NH1   | 2.44                     | 0.50              |
| 1:J:353:ASN:OD1 | 1:J:367:LYS:NZ   | 2.43                     | 0.50              |
| 1:N:245:ASP:HB2 | 1:N:307:LYS:HD3  | 1.93                     | 0.50              |
| 1:O:318:LYS:HG3 | 1:O:322:ARG:HH21 | 1.76                     | 0.50              |
| 1:P:108:GLY:O   | 1:P:130:TYR:OH   | 2.28                     | 0.50              |
| 1:A:227:MET:HE2 | 1:A:323:LYS:HG3  | 1.94                     | 0.49              |
| 1:J:83:ALA:HB1  | 1:J:98:ALA:HB1   | 1.94                     | 0.49              |
| 1:A:245:ASP:HB3 | 1:A:307:LYS:HD3  | 1.94                     | 0.49              |
| 1:D:115:TYR:HE2 | 1:D:334:GLU:HB2  | 1.78                     | 0.49              |
| 1:E:41:ASP:OD2  | 1:E:156:ASN:ND2  | 2.38                     | 0.49              |
| 1:I:1:MET:HB3   | 1:M:34:ASN:HB3   | 1.94                     | 0.49              |
| 1:I:23:ARG:NH2  | 1:I:37:ASP:OD1   | 2.45                     | 0.49              |
| 1:N:36:GLN:HB2  | 1:N:39:MET:HB2   | 1.94                     | 0.49              |
| 1:C:341:PHE:HZ  | 1:C:368:THR:HG23 | 1.77                     | 0.49              |
| 1:K:218:ASP:OD2 | 2:K:501:DGT:O3'  | 2.26                     | 0.49              |
| 1:P:236:GLU:OE1 | 1:P:322:ARG:NH1  | 2.45                     | 0.49              |
| 1:J:131:GLU:HG2 | 1:J:133:ASN:H    | 1.78                     | 0.49              |
| 1:M:64:ASP:HB3  | 1:M:67:LYS:HG3   | 1.95                     | 0.49              |
| 1:A:102:SER:O   | 1:A:105:HIS:ND1  | 2.38                     | 0.49              |
| 1:A:280:GLU:OE2 | 1:E:31:ARG:NH1   | 2.45                     | 0.49              |
| 1:O:133:ASN:ND2 | 2:O:501:DGT:O1G  | 2.45                     | 0.49              |
| 1:G:341:PHE:HZ  | 1:G:368:THR:HG23 | 1.78                     | 0.49              |
| 1:K:131:GLU:HG2 | 1:K:133:ASN:H    | 1.77                     | 0.49              |
| 1:O:55:GLN:O    | 1:O:71:ASN:ND2   | 2.43                     | 0.49              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:O:256:GLU:HB2 | 1:O:284:MET:HE1  | 1.93                     | 0.49              |
| 1:A:241:ASP:OD1 | 1:A:242:LYS:N    | 2.46                     | 0.49              |
| 1:G:50:SER:OG   | 1:G:144:GLU:OE2  | 2.20                     | 0.49              |
| 1:N:83:ALA:HB1  | 1:N:98:ALA:HB1   | 1.95                     | 0.49              |
| 1:P:341:PHE:HZ  | 1:P:368:THR:HG23 | 1.77                     | 0.49              |
| 1:N:64:ASP:HB3  | 1:N:67:LYS:HG3   | 1.95                     | 0.48              |
| 1:A:61:LEU:HD12 | 1:A:69:ASN:HD21  | 1.78                     | 0.48              |
| 1:G:321:LEU:O   | 1:G:327:GLN:NE2  | 2.46                     | 0.48              |
| 1:G:70:ARG:HG3  | 1:G:217:HIS:CD2  | 2.46                     | 0.48              |
| 1:N:241:ASP:OD1 | 1:N:241:ASP:N    | 2.46                     | 0.48              |
| 1:I:214:TYR:CE1 | 1:I:313:LYS:HG3  | 2.48                     | 0.48              |
| 1:H:214:TYR:HA  | 1:H:217:HIS:CD2  | 2.49                     | 0.48              |
| 1:M:131:GLU:HG2 | 1:M:133:ASN:H    | 1.78                     | 0.48              |
| 1:D:227:MET:HE2 | 1:D:323:LYS:HG3  | 1.94                     | 0.48              |
| 1:J:56:GLY:HA3  | 1:J:379:MET:HE2  | 1.95                     | 0.48              |
| 1:L:61:LEU:HB2  | 1:L:69:ASN:HD21  | 1.78                     | 0.48              |
| 1:O:307:LYS:O   | 1:O:311:GLY:N    | 2.38                     | 0.48              |
| 1:E:346:ASP:HB3 | 1:E:349:TYR:HB3  | 1.95                     | 0.48              |
| 1:O:213:ALA:C   | 1:O:217:HIS:HD1  | 2.21                     | 0.48              |
| 1:C:50:SER:OG   | 1:C:144:GLU:OE1  | 2.25                     | 0.48              |
| 1:C:102:SER:O   | 1:C:105:HIS:ND1  | 2.41                     | 0.48              |
| 1:D:60:LEU:HG   | 1:D:61:LEU:HD12  | 1.96                     | 0.48              |
| 1:G:318:LYS:O   | 1:G:322:ARG:HG3  | 2.14                     | 0.48              |
| 1:H:346:ASP:HB3 | 1:H:349:TYR:HB3  | 1.96                     | 0.48              |
| 1:K:64:ASP:HB3  | 1:K:67:LYS:HB2   | 1.95                     | 0.48              |
| 1:P:58:MET:HG3  | 1:P:62:GLY:HA2   | 1.94                     | 0.48              |
| 1:P:353:ASN:OD1 | 1:P:367:LYS:NZ   | 2.47                     | 0.48              |
| 1:B:227:MET:HE2 | 1:B:323:LYS:HG3  | 1.95                     | 0.47              |
| 1:C:115:TYR:HE2 | 1:C:334:GLU:HB2  | 1.79                     | 0.47              |
| 1:D:65:ALA:O    | 1:F:381:SER:OG   | 2.24                     | 0.47              |
| 1:G:102:SER:O   | 1:G:105:HIS:ND1  | 2.39                     | 0.47              |
| 1:I:139:ILE:HA  | 1:I:143:LEU:HB2  | 1.96                     | 0.47              |
| 1:M:110:PRO:HB3 | 1:M:120:LEU:HD12 | 1.96                     | 0.47              |
| 1:G:108:GLY:O   | 1:G:130:TYR:OH   | 2.26                     | 0.47              |
| 1:I:314:LYS:HA  | 1:I:317:PHE:CE1  | 2.50                     | 0.47              |
| 1:P:214:TYR:HE2 | 1:P:313:LYS:HG3  | 1.80                     | 0.47              |
| 1:I:256:GLU:HB2 | 1:I:284:MET:HE1  | 1.97                     | 0.47              |
| 1:N:110:PRO:HB3 | 1:N:120:LEU:HD12 | 1.97                     | 0.47              |
| 1:C:61:LEU:HD12 | 1:C:69:ASN:HD21  | 1.80                     | 0.47              |
| 1:J:108:GLY:O   | 1:J:130:TYR:OH   | 2.30                     | 0.47              |
| 1:K:319:ALA:HA  | 1:K:322:ARG:HD2  | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:108:GLY:O    | 1:M:130:TYR:OH   | 2.31                     | 0.47              |
| 1:A:115:TYR:HE2  | 1:A:334:GLU:HB2  | 1.80                     | 0.47              |
| 1:D:218:ASP:OD2  | 2:D:501:DGT:O3'  | 2.24                     | 0.47              |
| 1:F:346:ASP:HB3  | 1:F:349:TYR:HB3  | 1.95                     | 0.47              |
| 1:K:244:LYS:HD2  | 1:K:244:LYS:O    | 2.15                     | 0.47              |
| 1:M:168:PHE:O    | 1:M:178:LEU:N    | 2.43                     | 0.47              |
| 1:J:84:ARG:NH2   | 1:J:99:GLU:OE2   | 2.47                     | 0.47              |
| 1:O:222:ALA:HB1  | 1:O:228:ILE:HG22 | 1.97                     | 0.47              |
| 1:A:320:ILE:HG22 | 1:A:326:ILE:HG13 | 1.96                     | 0.47              |
| 1:L:55:GLN:O     | 1:L:71:ASN:ND2   | 2.45                     | 0.47              |
| 1:O:321:LEU:HD21 | 2:O:501:DGT:N1   | 2.30                     | 0.47              |
| 1:H:21:GLU:OE2   | 1:H:158:ARG:NH1  | 2.48                     | 0.46              |
| 1:K:23:ARG:NH1   | 1:K:154:ASN:O    | 2.47                     | 0.46              |
| 1:P:56:GLY:HA3   | 1:P:379:MET:HE2  | 1.97                     | 0.46              |
| 1:A:110:PRO:HB3  | 1:A:120:LEU:HD12 | 1.96                     | 0.46              |
| 1:A:269:THR:HB   | 1:F:322:ARG:HH12 | 1.80                     | 0.46              |
| 1:D:74:THR:HG21  | 1:F:52:ARG:HD2   | 1.96                     | 0.46              |
| 1:E:222:ALA:HB2  | 1:E:320:ILE:HD11 | 1.98                     | 0.46              |
| 1:F:197:VAL:HG22 | 1:F:199:LYS:H    | 1.80                     | 0.46              |
| 1:F:214:TYR:HE1  | 1:F:313:LYS:HG2  | 1.80                     | 0.46              |
| 1:H:10:ALA:HB1   | 1:H:92:LEU:HD21  | 1.97                     | 0.46              |
| 1:L:218:ASP:OD2  | 2:L:501:DGT:O3'  | 2.28                     | 0.46              |
| 1:O:330:GLU:OE2  | 2:O:501:DGT:N1   | 2.49                     | 0.46              |
| 1:C:70:ARG:NE    | 1:C:78:GLU:OE2   | 2.46                     | 0.46              |
| 1:D:35:ARG:HH21  | 1:D:40:ARG:HG2   | 1.80                     | 0.46              |
| 1:D:70:ARG:NE    | 1:D:78:GLU:OE1   | 2.48                     | 0.46              |
| 1:G:214:TYR:HB2  | 1:G:218:ASP:OD2  | 2.15                     | 0.46              |
| 1:I:106:ASP:OD1  | 1:I:109:ASN:ND2  | 2.47                     | 0.46              |
| 1:J:165:LYS:HD2  | 1:J:206:MET:HE1  | 1.97                     | 0.46              |
| 1:L:266:ARG:HH22 | 1:N:151:PRO:HB3  | 1.80                     | 0.46              |
| 1:M:353:ASN:OD1  | 1:M:367:LYS:NZ   | 2.48                     | 0.46              |
| 1:P:318:LYS:O    | 1:P:322:ARG:HG3  | 2.15                     | 0.46              |
| 1:G:266:ARG:NH1  | 1:H:148:TYR:O    | 2.48                     | 0.46              |
| 1:N:341:PHE:HZ   | 1:N:368:THR:HG23 | 1.80                     | 0.46              |
| 1:I:102:SER:O    | 1:I:105:HIS:ND1  | 2.44                     | 0.46              |
| 1:O:3:ASP:OD2    | 1:O:303:LYS:NZ   | 2.35                     | 0.46              |
| 1:B:21:GLU:OE2   | 1:B:158:ARG:NH1  | 2.48                     | 0.46              |
| 1:D:318:LYS:O    | 1:D:322:ARG:HG3  | 2.15                     | 0.46              |
| 1:D:346:ASP:HB3  | 1:D:349:TYR:HB3  | 1.98                     | 0.46              |
| 1:G:346:ASP:HB3  | 1:G:349:TYR:HB3  | 1.97                     | 0.46              |
| 1:H:320:ILE:HG22 | 1:H:326:ILE:HG13 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:330:GLU:OE2  | 2:I:501:DGT:N2   | 2.33                     | 0.46              |
| 1:K:318:LYS:O    | 1:K:322:ARG:HG3  | 2.16                     | 0.46              |
| 1:L:106:ASP:CB   | 1:L:109:ASN:HD22 | 2.28                     | 0.46              |
| 1:L:106:ASP:CG   | 1:L:109:ASN:ND2  | 2.73                     | 0.46              |
| 1:A:148:TYR:O    | 1:E:266:ARG:NH1  | 2.49                     | 0.46              |
| 1:L:364:ASN:O    | 1:L:365:ASP:OD1  | 2.34                     | 0.46              |
| 1:G:110:PRO:HB3  | 1:G:120:LEU:HD12 | 1.98                     | 0.46              |
| 1:J:330:GLU:OE2  | 2:J:501:DGT:N2   | 2.49                     | 0.46              |
| 1:H:127:CYS:SG   | 1:H:368:THR:HB   | 2.56                     | 0.46              |
| 1:I:222:ALA:HB1  | 1:I:228:ILE:HG22 | 1.97                     | 0.46              |
| 1:L:353:ASN:OD1  | 1:L:367:LYS:NZ   | 2.45                     | 0.46              |
| 1:P:168:PHE:O    | 1:P:178:LEU:N    | 2.45                     | 0.46              |
| 1:B:13:GLN:O     | 1:B:17:ILE:HG12  | 2.16                     | 0.45              |
| 1:D:17:ILE:HG23  | 1:D:20:LEU:HD12  | 1.99                     | 0.45              |
| 1:I:32:SER:HB3   | 1:I:40:ARG:HH12  | 1.82                     | 0.45              |
| 1:E:115:TYR:HE2  | 1:E:334:GLU:HB2  | 1.81                     | 0.45              |
| 1:F:341:PHE:HZ   | 1:F:368:THR:HG23 | 1.81                     | 0.45              |
| 1:G:214:TYR:CE2  | 1:G:313:LYS:HG2  | 2.48                     | 0.45              |
| 1:C:10:ALA:HB1   | 1:C:92:LEU:HD21  | 1.98                     | 0.45              |
| 1:D:317:PHE:CZ   | 1:D:321:LEU:HD13 | 2.52                     | 0.45              |
| 1:N:131:GLU:HG2  | 1:N:133:ASN:H    | 1.82                     | 0.45              |
| 1:C:105:HIS:NE2  | 1:C:106:ASP:OD2  | 2.50                     | 0.45              |
| 1:E:197:VAL:HG22 | 1:E:199:LYS:H    | 1.82                     | 0.45              |
| 1:K:289:LEU:HD22 | 1:K:309:ALA:HB2  | 1.97                     | 0.45              |
| 1:M:35:ARG:NH1   | 1:M:40:ARG:HG2   | 2.31                     | 0.45              |
| 1:A:105:HIS:NE2  | 1:A:106:ASP:OD2  | 2.48                     | 0.45              |
| 1:A:139:ILE:HA   | 1:A:143:LEU:HB2  | 1.99                     | 0.45              |
| 1:E:83:ALA:HB1   | 1:E:98:ALA:HB1   | 1.97                     | 0.45              |
| 1:I:110:PRO:HB3  | 1:I:120:LEU:HD12 | 1.99                     | 0.45              |
| 1:L:222:ALA:HB1  | 1:L:228:ILE:HG22 | 1.98                     | 0.45              |
| 1:L:341:PHE:HZ   | 1:L:368:THR:HG23 | 1.82                     | 0.45              |
| 1:J:110:PRO:HB3  | 1:J:120:LEU:HD12 | 1.97                     | 0.45              |
| 1:A:310:GLU:OE2  | 1:A:314:LYS:NZ   | 2.48                     | 0.45              |
| 1:C:197:VAL:HG22 | 1:C:199:LYS:H    | 1.82                     | 0.45              |
| 1:D:40:ARG:NH2   | 3:D:502:D5M:O2P  | 2.50                     | 0.45              |
| 1:D:105:HIS:NE2  | 1:D:210:ASP:OD1  | 2.49                     | 0.45              |
| 1:D:110:PRO:HB3  | 1:D:120:LEU:HD12 | 1.97                     | 0.45              |
| 1:D:129:GLY:O    | 1:D:369:ARG:NH2  | 2.41                     | 0.45              |
| 1:F:59:GLN:OE1   | 1:F:72:ARG:NH1   | 2.50                     | 0.45              |
| 1:H:341:PHE:HZ   | 1:H:368:THR:HG23 | 1.81                     | 0.45              |
| 1:M:245:ASP:HB2  | 1:M:307:LYS:HD3  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:70:ARG:NE    | 1:N:78:GLU:OE2   | 2.49                     | 0.45              |
| 1:P:23:ARG:NH2   | 1:P:37:ASP:OD1   | 2.50                     | 0.45              |
| 3:P:502:D5M:H8   | 3:P:502:D5M:H2'2 | 1.82                     | 0.45              |
| 1:B:230:LEU:HD12 | 1:B:233:ILE:HD11 | 1.98                     | 0.45              |
| 1:C:346:ASP:HB3  | 1:C:349:TYR:HB3  | 1.99                     | 0.45              |
| 1:I:317:PHE:HD2  | 1:I:321:LEU:HD13 | 1.82                     | 0.45              |
| 1:L:23:ARG:NH1   | 1:L:154:ASN:O    | 2.48                     | 0.45              |
| 1:L:139:ILE:HA   | 1:L:143:LEU:HB2  | 1.98                     | 0.45              |
| 1:E:70:ARG:NE    | 1:E:78:GLU:OE2   | 2.50                     | 0.45              |
| 1:E:349:TYR:O    | 1:F:331:ARG:NH2  | 2.47                     | 0.45              |
| 1:K:341:PHE:HZ   | 1:K:368:THR:HG23 | 1.81                     | 0.45              |
| 1:D:101:ALA:O    | 1:D:105:HIS:HB3  | 2.17                     | 0.44              |
| 1:G:101:ALA:O    | 1:G:105:HIS:HB3  | 2.17                     | 0.44              |
| 1:G:105:HIS:NE2  | 1:G:106:ASP:OD2  | 2.51                     | 0.44              |
| 1:O:279:LYS:NZ   | 1:P:144:GLU:OE2  | 2.50                     | 0.44              |
| 1:E:23:ARG:NH1   | 1:E:154:ASN:O    | 2.46                     | 0.44              |
| 3:E:502:D5M:H8   | 3:E:502:D5M:H2'2 | 1.83                     | 0.44              |
| 1:H:318:LYS:O    | 1:H:322:ARG:HG3  | 2.18                     | 0.44              |
| 1:J:36:GLN:O     | 1:J:40:ARG:HG3   | 2.16                     | 0.44              |
| 1:G:31:ARG:NH1   | 1:H:283:SER:HB3  | 2.33                     | 0.44              |
| 1:J:64:ASP:HB3   | 1:J:67:LYS:HB2   | 2.00                     | 0.44              |
| 1:P:227:MET:HE2  | 1:P:323:LYS:HG3  | 2.00                     | 0.44              |
| 1:G:245:ASP:HB3  | 1:G:307:LYS:HD3  | 1.98                     | 0.44              |
| 1:J:222:ALA:HB2  | 1:J:320:ILE:HD11 | 2.00                     | 0.44              |
| 1:P:378:MET:HG2  | 1:P:382:TYR:HD2  | 1.83                     | 0.44              |
| 1:B:348:LYS:HB3  | 1:B:348:LYS:HE3  | 1.63                     | 0.44              |
| 1:C:110:PRO:HB3  | 1:C:120:LEU:HD12 | 1.98                     | 0.44              |
| 1:D:83:ALA:HB1   | 1:D:98:ALA:HB1   | 2.00                     | 0.44              |
| 1:D:330:GLU:OE1  | 2:D:501:DGT:N2   | 2.44                     | 0.44              |
| 1:F:227:MET:HE2  | 1:F:323:LYS:HG3  | 1.98                     | 0.44              |
| 1:H:230:LEU:HD12 | 1:H:233:ILE:HD11 | 2.00                     | 0.44              |
| 1:M:150:TYR:CG   | 1:M:154:ASN:HB2  | 2.53                     | 0.44              |
| 1:N:165:LYS:HD2  | 1:N:206:MET:HE1  | 2.00                     | 0.44              |
| 1:I:318:LYS:HE2  | 1:I:322:ARG:HH21 | 1.82                     | 0.44              |
| 1:O:59:GLN:HE22  | 1:O:214:TYR:HE1  | 1.66                     | 0.44              |
| 1:J:31:ARG:NH1   | 1:K:280:GLU:OE2  | 2.50                     | 0.44              |
| 1:M:36:GLN:O     | 1:M:40:ARG:HG3   | 2.18                     | 0.44              |
| 1:P:23:ARG:NH1   | 1:P:154:ASN:O    | 2.50                     | 0.44              |
| 1:A:101:ALA:O    | 1:A:105:HIS:HB3  | 2.18                     | 0.44              |
| 1:G:41:ASP:OD2   | 1:G:156:ASN:ND2  | 2.32                     | 0.44              |
| 1:G:176:LYS:NZ   | 2:G:501:DGT:O2G  | 2.46                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:314:LYS:HA   | 1:I:317:PHE:HE1  | 1.82                     | 0.44              |
| 1:M:271:GLU:O    | 1:M:275:ILE:HG12 | 2.18                     | 0.44              |
| 1:M:314:LYS:HA   | 1:M:317:PHE:CE1  | 2.53                     | 0.44              |
| 1:M:357:PRO:HD2  | 1:M:360:LEU:HD12 | 1.98                     | 0.44              |
| 1:I:269:THR:HG22 | 1:N:322:ARG:HH21 | 1.83                     | 0.43              |
| 1:O:318:LYS:HE2  | 1:O:322:ARG:NH2  | 2.33                     | 0.43              |
| 1:F:10:ALA:HB1   | 1:F:92:LEU:HD21  | 2.00                     | 0.43              |
| 1:K:4:SER:O      | 1:K:8:GLU:HG2    | 2.17                     | 0.43              |
| 1:L:127:CYS:SG   | 1:L:369:ARG:HB2  | 2.58                     | 0.43              |
| 1:L:319:ALA:HA   | 1:L:322:ARG:HD2  | 2.00                     | 0.43              |
| 1:M:105:HIS:NE2  | 1:M:106:ASP:OD2  | 2.51                     | 0.43              |
| 3:G:502:D5M:H8   | 3:G:502:D5M:H2'2 | 1.84                     | 0.43              |
| 1:H:353:ASN:OD1  | 1:H:367:LYS:NZ   | 2.40                     | 0.43              |
| 1:O:4:SER:O      | 1:O:8:GLU:HG2    | 2.17                     | 0.43              |
| 1:O:61:LEU:HB2   | 1:O:69:ASN:HD21  | 1.83                     | 0.43              |
| 1:P:131:GLU:HG2  | 1:P:133:ASN:H    | 1.82                     | 0.43              |
| 1:P:145:LYS:NZ   | 1:P:151:PRO:HA   | 2.33                     | 0.43              |
| 1:J:341:PHE:HZ   | 1:J:368:THR:HG23 | 1.83                     | 0.43              |
| 1:L:322:ARG:HH12 | 1:P:270:SER:H    | 1.65                     | 0.43              |
| 1:A:313:LYS:O    | 1:A:317:PHE:HD1  | 2.00                     | 0.43              |
| 3:B:502:D5M:H8   | 3:B:502:D5M:H2'2 | 1.90                     | 0.43              |
| 1:C:317:PHE:HD2  | 1:C:321:LEU:HD13 | 1.84                     | 0.43              |
| 1:D:105:HIS:NE2  | 1:D:106:ASP:OD2  | 2.51                     | 0.43              |
| 1:G:115:TYR:HE2  | 1:G:334:GLU:HB2  | 1.83                     | 0.43              |
| 1:I:4:SER:O      | 1:I:8:GLU:HG2    | 2.17                     | 0.43              |
| 3:N:502:D5M:H8   | 3:N:502:D5M:H2'2 | 1.81                     | 0.43              |
| 1:P:105:HIS:NE2  | 1:P:106:ASP:OD2  | 2.52                     | 0.43              |
| 1:K:344:TYR:O    | 1:K:367:LYS:HE3  | 2.18                     | 0.43              |
| 1:A:54:LEU:HD11  | 1:A:107:ILE:HG22 | 2.01                     | 0.43              |
| 1:A:83:ALA:HB1   | 1:A:98:ALA:HB1   | 2.01                     | 0.43              |
| 1:A:214:TYR:HB2  | 1:A:218:ASP:OD1  | 2.19                     | 0.43              |
| 1:A:346:ASP:HB3  | 1:A:349:TYR:HB3  | 2.00                     | 0.43              |
| 1:G:54:LEU:HD11  | 1:G:107:ILE:HG22 | 2.01                     | 0.43              |
| 1:K:139:ILE:HA   | 1:K:143:LEU:HB2  | 1.99                     | 0.43              |
| 1:L:227:MET:HE2  | 1:L:323:LYS:HG3  | 2.00                     | 0.43              |
| 1:O:121:ASN:O    | 1:O:125:LEU:HG   | 2.18                     | 0.43              |
| 1:P:330:GLU:OE1  | 2:P:501:DGT:N2   | 2.52                     | 0.43              |
| 1:A:108:GLY:O    | 1:A:130:TYR:OH   | 2.30                     | 0.43              |
| 1:D:77:LEU:HD11  | 1:F:77:LEU:HD11  | 2.01                     | 0.43              |
| 1:I:169:ASN:OD1  | 1:I:172:GLN:HG3  | 2.19                     | 0.43              |
| 1:J:105:HIS:NE2  | 1:J:106:ASP:OD2  | 2.51                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:54:LEU:HD11 | 1:C:107:ILE:HG22 | 2.00                     | 0.43              |
| 1:E:60:LEU:HD21 | 1:E:320:ILE:HD12 | 2.01                     | 0.43              |
| 1:F:13:GLN:O    | 1:F:17:ILE:HG12  | 2.19                     | 0.43              |
| 1:F:58:MET:HG3  | 1:F:62:GLY:HA2   | 2.00                     | 0.43              |
| 1:H:227:MET:HE2 | 1:H:323:LYS:HG3  | 2.00                     | 0.43              |
| 1:I:318:LYS:HE2 | 1:I:322:ARG:NH2  | 2.34                     | 0.43              |
| 1:L:106:ASP:CA  | 1:L:109:ASN:HD22 | 2.30                     | 0.43              |
| 1:C:314:LYS:HA  | 1:C:317:PHE:CE1  | 2.54                     | 0.43              |
| 1:J:357:PRO:HD2 | 1:J:360:LEU:HD12 | 2.00                     | 0.43              |
| 1:B:127:CYS:SG  | 1:B:368:THR:HB   | 2.59                     | 0.42              |
| 1:H:36:GLN:O    | 1:H:40:ARG:HG3   | 2.18                     | 0.42              |
| 1:J:17:ILE:HD11 | 1:J:197:VAL:HG21 | 1.99                     | 0.42              |
| 1:K:9:TYR:CG    | 1:K:295:LEU:HD21 | 2.53                     | 0.42              |
| 1:L:9:TYR:CG    | 1:L:295:LEU:HD21 | 2.54                     | 0.42              |
| 3:M:502:D5M:H8  | 3:M:502:D5M:H2'2 | 1.87                     | 0.42              |
| 1:N:108:GLY:O   | 1:N:130:TYR:OH   | 2.30                     | 0.42              |
| 1:N:292:ASP:OD1 | 1:N:304:ARG:HG2  | 2.19                     | 0.42              |
| 1:P:83:ALA:HB1  | 1:P:98:ALA:HB1   | 2.01                     | 0.42              |
| 1:A:17:ILE:HG23 | 1:A:20:LEU:HD12  | 2.01                     | 0.42              |
| 1:B:133:ASN:ND2 | 2:B:501:DGT:O1G  | 2.52                     | 0.42              |
| 1:D:102:SER:O   | 1:D:105:HIS:ND1  | 2.40                     | 0.42              |
| 1:F:50:SER:OG   | 1:F:144:GLU:OE2  | 2.34                     | 0.42              |
| 1:F:102:SER:O   | 1:F:105:HIS:ND1  | 2.45                     | 0.42              |
| 1:J:40:ARG:NH2  | 3:J:502:D5M:O2P  | 2.49                     | 0.42              |
| 1:B:104:ALA:HB1 | 1:B:140:LEU:HD11 | 2.00                     | 0.42              |
| 1:E:91:GLU:OE2  | 1:E:91:GLU:HA    | 2.19                     | 0.42              |
| 1:J:168:PHE:O   | 1:J:178:LEU:N    | 2.46                     | 0.42              |
| 1:N:105:HIS:NE2 | 1:N:106:ASP:OD2  | 2.52                     | 0.42              |
| 1:B:10:ALA:HB1  | 1:B:92:LEU:HD21  | 2.00                     | 0.42              |
| 1:C:101:ALA:O   | 1:C:105:HIS:HB3  | 2.18                     | 0.42              |
| 1:C:245:ASP:HB3 | 1:C:307:LYS:HD3  | 2.01                     | 0.42              |
| 1:E:101:ALA:HA  | 1:E:163:ILE:HG22 | 2.01                     | 0.42              |
| 1:I:214:TYR:HB2 | 1:I:218:ASP:OD2  | 2.20                     | 0.42              |
| 1:O:127:CYS:SG  | 1:O:368:THR:HB   | 2.59                     | 0.42              |
| 1:B:36:GLN:O    | 1:B:40:ARG:HG3   | 2.20                     | 0.42              |
| 1:D:54:LEU:HD11 | 1:D:107:ILE:HG22 | 2.02                     | 0.42              |
| 1:E:127:CYS:SG  | 1:E:368:THR:HB   | 2.60                     | 0.42              |
| 1:F:58:MET:HB3  | 1:F:113:GLY:N    | 2.34                     | 0.42              |
| 1:K:222:ALA:HB1 | 1:K:228:ILE:HG22 | 2.01                     | 0.42              |
| 1:L:102:SER:O   | 1:L:105:HIS:ND1  | 2.46                     | 0.42              |
| 1:O:305:HIS:HB3 | 1:O:308:LEU:HB3  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:502:D5M:HB8  | 3:A:502:D5M:H2'2 | 1.84                     | 0.42              |
| 1:B:168:PHE:O    | 1:B:178:LEU:N    | 2.48                     | 0.42              |
| 1:P:64:ASP:HB3   | 1:P:67:LYS:HB2   | 2.01                     | 0.42              |
| 1:G:222:ALA:HB1  | 1:G:228:ILE:HG22 | 2.02                     | 0.42              |
| 1:I:60:LEU:HD21  | 1:I:320:ILE:HD12 | 2.01                     | 0.42              |
| 1:L:121:ASN:O    | 1:L:125:LEU:HG   | 2.19                     | 0.42              |
| 1:P:110:PRO:HB3  | 1:P:120:LEU:HD12 | 2.00                     | 0.42              |
| 1:E:114:ALA:HB3  | 2:E:501:DGT:C5   | 2.49                     | 0.42              |
| 1:M:83:ALA:HB1   | 1:M:98:ALA:HB1   | 2.01                     | 0.42              |
| 1:M:378:MET:HG2  | 1:M:382:TYR:HD2  | 1.84                     | 0.42              |
| 1:N:139:ILE:HG12 | 1:N:143:LEU:HD12 | 2.00                     | 0.42              |
| 1:P:314:LYS:HA   | 1:P:317:PHE:CE1  | 2.55                     | 0.42              |
| 1:A:31:ARG:NH2   | 1:E:280:GLU:OE2  | 2.53                     | 0.42              |
| 1:A:222:ALA:HB1  | 1:A:228:ILE:HG22 | 2.02                     | 0.42              |
| 1:D:41:ASP:OD2   | 1:D:156:ASN:ND2  | 2.31                     | 0.42              |
| 1:E:330:GLU:OE2  | 2:E:501:DGT:N2   | 2.48                     | 0.42              |
| 1:F:115:TYR:HE2  | 1:F:334:GLU:HB2  | 1.85                     | 0.42              |
| 1:K:35:ARG:NH1   | 3:K:502:D5M:O3P  | 2.53                     | 0.42              |
| 1:A:278:LYS:HE2  | 1:A:278:LYS:HB2  | 1.74                     | 0.42              |
| 1:A:330:GLU:OE2  | 2:A:501:DGT:N2   | 2.37                     | 0.42              |
| 2:I:501:DGT:H8   | 2:I:501:DGT:H2'A | 1.80                     | 0.42              |
| 1:M:35:ARG:HH12  | 1:M:40:ARG:HG2   | 1.85                     | 0.42              |
| 1:P:36:GLN:O     | 1:P:40:ARG:HG3   | 2.20                     | 0.42              |
| 1:F:139:ILE:HA   | 1:F:143:LEU:HB2  | 2.02                     | 0.41              |
| 1:H:105:HIS:NE2  | 1:H:106:ASP:OD2  | 2.53                     | 0.41              |
| 1:K:304:ARG:NH1  | 1:K:304:ARG:HB2  | 2.35                     | 0.41              |
| 1:L:52:ARG:NH1   | 1:N:68:PHE:O     | 2.53                     | 0.41              |
| 1:L:72:ARG:HD2   | 1:L:106:ASP:HB3  | 2.02                     | 0.41              |
| 1:P:40:ARG:NH2   | 3:P:502:D5M:O2P  | 2.47                     | 0.41              |
| 1:J:54:LEU:HD11  | 1:J:107:ILE:HG22 | 2.02                     | 0.41              |
| 1:L:4:SER:O      | 1:L:8:GLU:HG2    | 2.20                     | 0.41              |
| 1:J:314:LYS:HB3  | 1:J:318:LYS:HE3  | 2.02                     | 0.41              |
| 1:M:227:MET:HE2  | 1:M:323:LYS:HG3  | 2.02                     | 0.41              |
| 1:P:165:LYS:HD2  | 1:P:206:MET:HE1  | 2.02                     | 0.41              |
| 1:A:269:THR:HB   | 1:F:322:ARG:NH1  | 2.36                     | 0.41              |
| 1:B:60:LEU:HG    | 1:B:61:LEU:HD12  | 2.02                     | 0.41              |
| 1:B:270:SER:H    | 1:G:322:ARG:HH12 | 1.67                     | 0.41              |
| 1:C:108:GLY:O    | 1:C:130:TYR:OH   | 2.33                     | 0.41              |
| 1:D:40:ARG:HH21  | 3:D:502:D5M:P    | 2.43                     | 0.41              |
| 1:F:348:LYS:HE3  | 1:F:348:LYS:HB3  | 1.62                     | 0.41              |
| 1:G:235:HIS:CE1  | 1:G:239:ILE:HD13 | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:501:DGT:H2'A | 2:G:501:DGT:H8   | 1.76                     | 0.41              |
| 1:L:3:ASP:OD2    | 1:L:303:LYS:NZ   | 2.35                     | 0.41              |
| 1:L:214:TYR:HB2  | 1:L:218:ASP:OD2  | 2.20                     | 0.41              |
| 1:M:115:TYR:HB2  | 1:M:330:GLU:OE1  | 2.16                     | 0.41              |
| 2:A:501:DGT:H8   | 2:A:501:DGT:H2'A | 1.77                     | 0.41              |
| 1:D:75:HIS:O     | 1:D:79:VAL:HG23  | 2.20                     | 0.41              |
| 1:M:54:LEU:HD11  | 1:M:107:ILE:HG22 | 2.03                     | 0.41              |
| 1:M:169:ASN:OD1  | 1:M:172:GLN:HG3  | 2.21                     | 0.41              |
| 1:O:114:ALA:HB3  | 2:O:501:DGT:C5   | 2.50                     | 0.41              |
| 1:A:77:LEU:HD11  | 1:E:77:LEU:HD11  | 2.02                     | 0.41              |
| 1:D:222:ALA:HB1  | 1:D:228:ILE:HG22 | 2.03                     | 0.41              |
| 1:D:353:ASN:OD1  | 1:D:367:LYS:NZ   | 2.51                     | 0.41              |
| 1:E:319:ALA:HA   | 1:E:322:ARG:NE   | 2.35                     | 0.41              |
| 1:F:60:LEU:HG    | 1:F:61:LEU:HD12  | 2.02                     | 0.41              |
| 1:G:83:ALA:HB1   | 1:G:98:ALA:HB1   | 2.03                     | 0.41              |
| 1:J:331:ARG:HD2  | 1:P:349:TYR:CE1  | 2.56                     | 0.41              |
| 1:O:23:ARG:NH1   | 1:O:154:ASN:O    | 2.49                     | 0.41              |
| 1:O:341:PHE:HZ   | 1:O:368:THR:HG23 | 1.85                     | 0.41              |
| 1:C:83:ALA:HB1   | 1:C:98:ALA:HB1   | 2.02                     | 0.41              |
| 1:E:307:LYS:HA   | 1:E:310:GLU:HG2  | 2.02                     | 0.41              |
| 1:F:295:LEU:HD12 | 1:F:295:LEU:HA   | 1.88                     | 0.41              |
| 1:H:228:ILE:HG13 | 1:H:232:GLU:OE1  | 2.21                     | 0.41              |
| 1:J:292:ASP:OD1  | 1:J:304:ARG:HG2  | 2.20                     | 0.41              |
| 1:M:23:ARG:NH1   | 1:M:154:ASN:O    | 2.51                     | 0.41              |
| 1:N:354:MET:HB3  | 1:P:327:GLN:HE21 | 1.85                     | 0.41              |
| 1:P:54:LEU:HD11  | 1:P:107:ILE:HG22 | 2.02                     | 0.41              |
| 1:C:139:ILE:HA   | 1:C:143:LEU:HB2  | 2.03                     | 0.41              |
| 1:E:72:ARG:HD2   | 1:E:106:ASP:HB3  | 2.02                     | 0.41              |
| 1:H:104:ALA:HB1  | 1:H:140:LEU:HD11 | 2.03                     | 0.41              |
| 1:I:344:TYR:O    | 1:I:367:LYS:HE3  | 2.20                     | 0.41              |
| 1:K:305:HIS:HB3  | 1:K:308:LEU:HB3  | 2.02                     | 0.41              |
| 1:B:341:PHE:HZ   | 1:B:368:THR:HG23 | 1.85                     | 0.41              |
| 1:D:50:SER:OG    | 1:D:144:GLU:OE2  | 2.25                     | 0.41              |
| 1:D:241:ASP:OD1  | 1:D:242:LYS:N    | 2.53                     | 0.41              |
| 1:E:228:ILE:HG13 | 1:E:232:GLU:OE1  | 2.21                     | 0.41              |
| 1:G:214:TYR:HA   | 1:G:217:HIS:CE1  | 2.56                     | 0.41              |
| 1:G:258:GLN:O    | 1:G:262:MET:HG2  | 2.21                     | 0.41              |
| 1:H:102:SER:O    | 1:H:105:HIS:ND1  | 2.45                     | 0.41              |
| 1:I:304:ARG:NH1  | 1:I:304:ARG:HB2  | 2.35                     | 0.41              |
| 2:L:501:DGT:H8   | 2:L:501:DGT:H2'A | 1.80                     | 0.41              |
| 1:N:58:MET:HB3   | 1:N:113:GLY:N    | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:270:SER:H    | 1:H:322:ARG:HH12 | 1.68                     | 0.41              |
| 1:G:77:LEU:HD11  | 1:H:77:LEU:HD11  | 2.03                     | 0.41              |
| 1:M:341:PHE:HZ   | 1:M:368:THR:HG23 | 1.86                     | 0.41              |
| 1:N:323:LYS:HA   | 1:N:323:LYS:HD3  | 1.90                     | 0.41              |
| 1:D:327:GLN:OE1  | 1:G:354:MET:HB3  | 2.21                     | 0.40              |
| 1:E:13:GLN:O     | 1:E:17:ILE:HG12  | 2.21                     | 0.40              |
| 1:E:393:LYS:HE2  | 1:E:393:LYS:HB3  | 1.72                     | 0.40              |
| 1:G:56:GLY:HA3   | 1:G:379:MET:HE3  | 2.03                     | 0.40              |
| 1:J:214:TYR:OH   | 2:J:501:DGT:O2B  | 2.39                     | 0.40              |
| 1:L:60:LEU:HD21  | 1:L:320:ILE:HD12 | 2.03                     | 0.40              |
| 1:N:271:GLU:O    | 1:N:275:ILE:HG12 | 2.20                     | 0.40              |
| 1:N:321:LEU:HD12 | 1:N:327:GLN:NE2  | 2.36                     | 0.40              |
| 1:A:327:GLN:O    | 1:A:331:ARG:HG2  | 2.21                     | 0.40              |
| 1:E:58:MET:HB3   | 1:E:113:GLY:N    | 2.36                     | 0.40              |
| 1:E:320:ILE:HG22 | 1:E:326:ILE:HG13 | 2.03                     | 0.40              |
| 1:F:35:ARG:NH1   | 3:F:502:D5M:O3P  | 2.54                     | 0.40              |
| 1:I:254:ALA:O    | 1:I:258:GLN:HG3  | 2.22                     | 0.40              |
| 1:I:327:GLN:O    | 1:I:331:ARG:HG2  | 2.22                     | 0.40              |
| 1:L:40:ARG:HH21  | 3:L:502:D5M:P    | 2.44                     | 0.40              |
| 1:N:321:LEU:CD1  | 1:N:327:GLN:NE2  | 2.83                     | 0.40              |
| 1:P:150:TYR:CD2  | 1:P:154:ASN:HB2  | 2.56                     | 0.40              |
| 1:B:50:SER:OG    | 1:B:144:GLU:OE2  | 2.36                     | 0.40              |
| 1:C:40:ARG:HH21  | 3:C:502:D5M:P    | 2.45                     | 0.40              |
| 1:D:58:MET:HB3   | 1:D:113:GLY:N    | 2.37                     | 0.40              |
| 1:I:75:HIS:O     | 1:I:79:VAL:HG23  | 2.22                     | 0.40              |
| 1:K:102:SER:O    | 1:K:105:HIS:ND1  | 2.47                     | 0.40              |
| 1:P:241:ASP:OD1  | 1:P:241:ASP:N    | 2.43                     | 0.40              |
| 1:B:110:PRO:HB3  | 1:B:120:LEU:HD12 | 2.03                     | 0.40              |
| 1:D:133:ASN:ND2  | 2:D:501:DGT:O1G  | 2.46                     | 0.40              |
| 1:G:13:GLN:O     | 1:G:17:ILE:HG12  | 2.21                     | 0.40              |
| 1:G:40:ARG:HH21  | 3:G:502:D5M:P    | 2.44                     | 0.40              |
| 1:G:280:GLU:OE2  | 1:H:31:ARG:NH1   | 2.55                     | 0.40              |
| 1:H:168:PHE:O    | 1:H:178:LEU:N    | 2.51                     | 0.40              |
| 1:L:75:HIS:O     | 1:L:79:VAL:HG23  | 2.21                     | 0.40              |
| 1:N:357:PRO:HD2  | 1:N:360:LEU:HD12 | 2.04                     | 0.40              |

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 1   | A     | 400/402 (100%)   | 394 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 1   | B     | 400/402 (100%)   | 392 (98%)  | 8 (2%)   | 0        | 100         | 100 |
| 1   | C     | 400/402 (100%)   | 395 (99%)  | 5 (1%)   | 0        | 100         | 100 |
| 1   | D     | 400/402 (100%)   | 393 (98%)  | 7 (2%)   | 0        | 100         | 100 |
| 1   | E     | 400/402 (100%)   | 395 (99%)  | 5 (1%)   | 0        | 100         | 100 |
| 1   | F     | 400/402 (100%)   | 393 (98%)  | 7 (2%)   | 0        | 100         | 100 |
| 1   | G     | 400/402 (100%)   | 396 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 1   | H     | 400/402 (100%)   | 395 (99%)  | 5 (1%)   | 0        | 100         | 100 |
| 1   | I     | 400/402 (100%)   | 395 (99%)  | 5 (1%)   | 0        | 100         | 100 |
| 1   | J     | 400/402 (100%)   | 392 (98%)  | 8 (2%)   | 0        | 100         | 100 |
| 1   | K     | 400/402 (100%)   | 393 (98%)  | 7 (2%)   | 0        | 100         | 100 |
| 1   | L     | 400/402 (100%)   | 388 (97%)  | 12 (3%)  | 0        | 100         | 100 |
| 1   | M     | 400/402 (100%)   | 395 (99%)  | 5 (1%)   | 0        | 100         | 100 |
| 1   | N     | 400/402 (100%)   | 396 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 1   | O     | 400/402 (100%)   | 390 (98%)  | 10 (2%)  | 0        | 100         | 100 |
| 1   | P     | 400/402 (100%)   | 390 (98%)  | 10 (2%)  | 0        | 100         | 100 |
| All | All   | 6400/6432 (100%) | 6292 (98%) | 108 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.



| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 1   | A     | 344/344 (100%)   | 344 (100%)  | 0        | 100         | 100 |
| 1   | B     | 344/344 (100%)   | 344 (100%)  | 0        | 100         | 100 |
| 1   | C     | 344/344 (100%)   | 344 (100%)  | 0        | 100         | 100 |
| 1   | D     | 344/344 (100%)   | 344 (100%)  | 0        | 100         | 100 |
| 1   | E     | 344/344 (100%)   | 344 (100%)  | 0        | 100         | 100 |
| 1   | F     | 344/344 (100%)   | 344 (100%)  | 0        | 100         | 100 |
| 1   | G     | 344/344 (100%)   | 344 (100%)  | 0        | 100         | 100 |
| 1   | H     | 344/344 (100%)   | 344 (100%)  | 0        | 100         | 100 |
| 1   | I     | 344/344 (100%)   | 344 (100%)  | 0        | 100         | 100 |
| 1   | J     | 344/344 (100%)   | 344 (100%)  | 0        | 100         | 100 |
| 1   | K     | 344/344 (100%)   | 344 (100%)  | 0        | 100         | 100 |
| 1   | L     | 344/344 (100%)   | 344 (100%)  | 0        | 100         | 100 |
| 1   | M     | 344/344 (100%)   | 344 (100%)  | 0        | 100         | 100 |
| 1   | N     | 344/344 (100%)   | 344 (100%)  | 0        | 100         | 100 |
| 1   | O     | 344/344 (100%)   | 344 (100%)  | 0        | 100         | 100 |
| 1   | P     | 344/344 (100%)   | 344 (100%)  | 0        | 100         | 100 |
| All | All   | 5504/5504 (100%) | 5504 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 15  | ASN  |
| 1   | A     | 217 | HIS  |
| 1   | B     | 15  | ASN  |
| 1   | B     | 109 | ASN  |
| 1   | B     | 171 | HIS  |
| 1   | C     | 15  | ASN  |
| 1   | C     | 174 | ASN  |
| 1   | D     | 15  | ASN  |
| 1   | D     | 36  | GLN  |
| 1   | D     | 174 | ASN  |
| 1   | E     | 15  | ASN  |
| 1   | F     | 15  | ASN  |
| 1   | F     | 174 | ASN  |
| 1   | G     | 15  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 34  | ASN  |
| 1   | G     | 81  | GLN  |
| 1   | G     | 174 | ASN  |
| 1   | G     | 217 | HIS  |
| 1   | H     | 15  | ASN  |
| 1   | I     | 133 | ASN  |
| 1   | I     | 156 | ASN  |
| 1   | J     | 36  | GLN  |
| 1   | J     | 258 | GLN  |
| 1   | J     | 305 | HIS  |
| 1   | J     | 327 | GLN  |
| 1   | K     | 109 | ASN  |
| 1   | L     | 15  | ASN  |
| 1   | L     | 109 | ASN  |
| 1   | L     | 147 | HIS  |
| 1   | M     | 15  | ASN  |
| 1   | M     | 258 | GLN  |
| 1   | N     | 15  | ASN  |
| 1   | N     | 27  | HIS  |
| 1   | N     | 34  | ASN  |
| 1   | O     | 15  | ASN  |
| 1   | O     | 27  | HIS  |
| 1   | O     | 174 | ASN  |
| 1   | O     | 258 | GLN  |
| 1   | P     | 36  | GLN  |
| 1   | P     | 172 | GLN  |
| 1   | P     | 258 | GLN  |
| 1   | P     | 327 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

32 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | D5M  | A     | 502 | -    | 24,24,24     | 3.41 | 9 (37%)  | 36,36,36    | 2.43 | 11 (30%) |
| 2   | DGT  | L     | 501 | -    | 29,33,33     | 3.27 | 15 (51%) | 44,52,52    | 2.37 | 13 (29%) |
| 2   | DGT  | G     | 501 | -    | 29,33,33     | 3.28 | 15 (51%) | 44,52,52    | 2.37 | 14 (31%) |
| 2   | DGT  | E     | 501 | -    | 29,33,33     | 3.27 | 15 (51%) | 44,52,52    | 2.38 | 13 (29%) |
| 2   | DGT  | H     | 501 | -    | 29,33,33     | 3.29 | 16 (55%) | 44,52,52    | 2.36 | 13 (29%) |
| 2   | DGT  | I     | 501 | -    | 29,33,33     | 3.26 | 15 (51%) | 44,52,52    | 2.38 | 13 (29%) |
| 2   | DGT  | O     | 501 | -    | 29,33,33     | 3.23 | 15 (51%) | 44,52,52    | 2.27 | 13 (29%) |
| 3   | D5M  | G     | 502 | -    | 24,24,24     | 3.40 | 9 (37%)  | 36,36,36    | 2.42 | 11 (30%) |
| 3   | D5M  | I     | 502 | -    | 24,24,24     | 3.40 | 9 (37%)  | 36,36,36    | 2.41 | 12 (33%) |
| 2   | DGT  | P     | 501 | -    | 29,33,33     | 3.27 | 15 (51%) | 44,52,52    | 2.39 | 14 (31%) |
| 2   | DGT  | B     | 501 | -    | 29,33,33     | 3.23 | 15 (51%) | 44,52,52    | 2.27 | 13 (29%) |
| 3   | D5M  | E     | 502 | -    | 24,24,24     | 3.41 | 9 (37%)  | 36,36,36    | 2.43 | 13 (36%) |
| 2   | DGT  | K     | 501 | -    | 29,33,33     | 3.27 | 15 (51%) | 44,52,52    | 2.37 | 13 (29%) |
| 3   | D5M  | H     | 502 | -    | 24,24,24     | 3.39 | 9 (37%)  | 36,36,36    | 2.44 | 12 (33%) |
| 2   | DGT  | F     | 501 | -    | 29,33,33     | 3.28 | 15 (51%) | 44,52,52    | 2.38 | 13 (29%) |
| 3   | D5M  | N     | 502 | -    | 24,24,24     | 3.41 | 9 (37%)  | 36,36,36    | 2.41 | 13 (36%) |
| 3   | D5M  | C     | 502 | -    | 24,24,24     | 3.40 | 9 (37%)  | 36,36,36    | 2.44 | 12 (33%) |
| 3   | D5M  | D     | 502 | -    | 24,24,24     | 3.40 | 9 (37%)  | 36,36,36    | 2.44 | 12 (33%) |
| 2   | DGT  | J     | 501 | -    | 29,33,33     | 3.30 | 16 (55%) | 44,52,52    | 2.36 | 13 (29%) |
| 2   | DGT  | M     | 501 | -    | 29,33,33     | 3.27 | 15 (51%) | 44,52,52    | 2.38 | 13 (29%) |
| 3   | D5M  | J     | 502 | -    | 24,24,24     | 3.41 | 9 (37%)  | 36,36,36    | 2.43 | 12 (33%) |
| 3   | D5M  | M     | 502 | -    | 24,24,24     | 3.41 | 9 (37%)  | 36,36,36    | 2.44 | 11 (30%) |
| 2   | DGT  | D     | 501 | -    | 29,33,33     | 3.28 | 15 (51%) | 44,52,52    | 2.34 | 13 (29%) |
| 2   | DGT  | N     | 501 | -    | 29,33,33     | 3.27 | 15 (51%) | 44,52,52    | 2.38 | 13 (29%) |
| 3   | D5M  | L     | 502 | -    | 24,24,24     | 3.41 | 9 (37%)  | 36,36,36    | 2.42 | 10 (27%) |
| 2   | DGT  | C     | 501 | -    | 29,33,33     | 3.27 | 15 (51%) | 44,52,52    | 2.37 | 14 (31%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | D5M  | K     | 502 | -    | 24,24,24     | 3.40 | 9 (37%)  | 36,36,36    | 2.46 | 12 (33%) |
| 3   | D5M  | O     | 502 | -    | 24,24,24     | 3.40 | 9 (37%)  | 36,36,36    | 2.43 | 12 (33%) |
| 3   | D5M  | B     | 502 | -    | 24,24,24     | 3.41 | 9 (37%)  | 36,36,36    | 2.42 | 12 (33%) |
| 3   | D5M  | P     | 502 | -    | 24,24,24     | 3.41 | 9 (37%)  | 36,36,36    | 2.42 | 11 (30%) |
| 2   | DGT  | A     | 501 | -    | 29,33,33     | 3.27 | 15 (51%) | 44,52,52    | 2.38 | 13 (29%) |
| 3   | D5M  | F     | 502 | -    | 24,24,24     | 3.40 | 9 (37%)  | 36,36,36    | 2.45 | 12 (33%) |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | D5M  | A     | 502 | -    | -       | 5/10/22/22 | 0/3/3/3 |
| 2   | DGT  | L     | 501 | -    | -       | 4/22/34/34 | 0/3/3/3 |
| 2   | DGT  | G     | 501 | -    | -       | 4/22/34/34 | 0/3/3/3 |
| 2   | DGT  | E     | 501 | -    | -       | 9/22/34/34 | 0/3/3/3 |
| 2   | DGT  | H     | 501 | -    | -       | 8/22/34/34 | 0/3/3/3 |
| 2   | DGT  | I     | 501 | -    | -       | 3/22/34/34 | 0/3/3/3 |
| 2   | DGT  | O     | 501 | -    | -       | 6/22/34/34 | 0/3/3/3 |
| 3   | D5M  | G     | 502 | -    | -       | 5/10/22/22 | 0/3/3/3 |
| 3   | D5M  | I     | 502 | -    | -       | 2/10/22/22 | 0/3/3/3 |
| 2   | DGT  | P     | 501 | -    | -       | 3/22/34/34 | 0/3/3/3 |
| 2   | DGT  | B     | 501 | -    | -       | 6/22/34/34 | 0/3/3/3 |
| 3   | D5M  | E     | 502 | -    | -       | 5/10/22/22 | 0/3/3/3 |
| 2   | DGT  | K     | 501 | -    | -       | 8/22/34/34 | 0/3/3/3 |
| 3   | D5M  | H     | 502 | -    | -       | 5/10/22/22 | 0/3/3/3 |
| 2   | DGT  | F     | 501 | -    | -       | 9/22/34/34 | 0/3/3/3 |
| 3   | D5M  | N     | 502 | -    | -       | 3/10/22/22 | 0/3/3/3 |
| 3   | D5M  | C     | 502 | -    | -       | 5/10/22/22 | 0/3/3/3 |
| 3   | D5M  | D     | 502 | -    | -       | 4/10/22/22 | 0/3/3/3 |
| 2   | DGT  | J     | 501 | -    | -       | 8/22/34/34 | 0/3/3/3 |
| 2   | DGT  | M     | 501 | -    | -       | 9/22/34/34 | 0/3/3/3 |
| 3   | D5M  | J     | 502 | -    | -       | 3/10/22/22 | 0/3/3/3 |
| 3   | D5M  | M     | 502 | -    | -       | 5/10/22/22 | 0/3/3/3 |
| 2   | DGT  | D     | 501 | -    | -       | 4/22/34/34 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | DGT  | N     | 501 | -    | -       | 9/22/34/34 | 0/3/3/3 |
| 3   | D5M  | L     | 502 | -    | -       | 3/10/22/22 | 0/3/3/3 |
| 2   | DGT  | C     | 501 | -    | -       | 6/22/34/34 | 0/3/3/3 |
| 3   | D5M  | K     | 502 | -    | -       | 2/10/22/22 | 0/3/3/3 |
| 3   | D5M  | O     | 502 | -    | -       | 2/10/22/22 | 0/3/3/3 |
| 3   | D5M  | B     | 502 | -    | -       | 3/10/22/22 | 0/3/3/3 |
| 3   | D5M  | P     | 502 | -    | -       | 3/10/22/22 | 0/3/3/3 |
| 2   | DGT  | A     | 501 | -    | -       | 9/22/34/34 | 0/3/3/3 |
| 3   | D5M  | F     | 502 | -    | -       | 4/10/22/22 | 0/3/3/3 |

All (386) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | A     | 502 | D5M  | C3'-C4' | -9.05 | 1.28        | 1.53     |
| 3   | L     | 502 | D5M  | C3'-C4' | -9.03 | 1.28        | 1.53     |
| 3   | G     | 502 | D5M  | C3'-C4' | -9.03 | 1.28        | 1.53     |
| 3   | M     | 502 | D5M  | C3'-C4' | -9.03 | 1.28        | 1.53     |
| 3   | J     | 502 | D5M  | C3'-C4' | -9.01 | 1.28        | 1.53     |
| 3   | N     | 502 | D5M  | C3'-C4' | -9.00 | 1.28        | 1.53     |
| 3   | P     | 502 | D5M  | C3'-C4' | -9.00 | 1.28        | 1.53     |
| 3   | E     | 502 | D5M  | C3'-C4' | -8.99 | 1.28        | 1.53     |
| 3   | C     | 502 | D5M  | C3'-C4' | -8.98 | 1.28        | 1.53     |
| 3   | K     | 502 | D5M  | C3'-C4' | -8.96 | 1.28        | 1.53     |
| 3   | I     | 502 | D5M  | C3'-C4' | -8.94 | 1.28        | 1.53     |
| 3   | O     | 502 | D5M  | C3'-C4' | -8.94 | 1.28        | 1.53     |
| 3   | H     | 502 | D5M  | C3'-C4' | -8.92 | 1.28        | 1.53     |
| 3   | B     | 502 | D5M  | C3'-C4' | -8.86 | 1.28        | 1.53     |
| 3   | F     | 502 | D5M  | C3'-C4' | -8.85 | 1.28        | 1.53     |
| 3   | D     | 502 | D5M  | C3'-C4' | -8.85 | 1.28        | 1.53     |
| 2   | O     | 501 | DGT  | C2'-C3' | -7.93 | 1.31        | 1.52     |
| 2   | B     | 501 | DGT  | C2'-C3' | -7.93 | 1.31        | 1.52     |
| 2   | H     | 501 | DGT  | C2'-C3' | -7.90 | 1.32        | 1.52     |
| 2   | J     | 501 | DGT  | C2'-C3' | -7.90 | 1.32        | 1.52     |
| 2   | K     | 501 | DGT  | C2'-C3' | -7.88 | 1.32        | 1.52     |
| 2   | L     | 501 | DGT  | C2'-C3' | -7.88 | 1.32        | 1.52     |
| 2   | I     | 501 | DGT  | C2'-C3' | -7.81 | 1.32        | 1.52     |
| 2   | G     | 501 | DGT  | C2'-C3' | -7.81 | 1.32        | 1.52     |
| 2   | D     | 501 | DGT  | C2'-C3' | -7.80 | 1.32        | 1.52     |
| 2   | F     | 501 | DGT  | C2'-C3' | -7.75 | 1.32        | 1.52     |
| 2   | E     | 501 | DGT  | C2'-C3' | -7.75 | 1.32        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | A     | 501 | DGT  | C2'-C3' | -7.74 | 1.32        | 1.52     |
| 2   | N     | 501 | DGT  | C2'-C3' | -7.74 | 1.32        | 1.52     |
| 2   | C     | 501 | DGT  | C2'-C3' | -7.73 | 1.32        | 1.52     |
| 2   | P     | 501 | DGT  | C2'-C3' | -7.73 | 1.32        | 1.52     |
| 2   | M     | 501 | DGT  | C2'-C3' | -7.72 | 1.32        | 1.52     |
| 3   | B     | 502 | D5M  | C2'-C1' | -7.39 | 1.31        | 1.52     |
| 3   | D     | 502 | D5M  | C2'-C1' | -7.33 | 1.31        | 1.52     |
| 3   | F     | 502 | D5M  | C2'-C1' | -7.33 | 1.31        | 1.52     |
| 3   | P     | 502 | D5M  | C2'-C1' | -7.31 | 1.32        | 1.52     |
| 3   | N     | 502 | D5M  | C2'-C1' | -7.30 | 1.32        | 1.52     |
| 3   | O     | 502 | D5M  | C2'-C1' | -7.29 | 1.32        | 1.52     |
| 3   | M     | 502 | D5M  | C2'-C1' | -7.29 | 1.32        | 1.52     |
| 3   | E     | 502 | D5M  | C2'-C1' | -7.28 | 1.32        | 1.52     |
| 3   | I     | 502 | D5M  | C2'-C1' | -7.28 | 1.32        | 1.52     |
| 3   | J     | 502 | D5M  | C2'-C1' | -7.26 | 1.32        | 1.52     |
| 3   | H     | 502 | D5M  | C2'-C1' | -7.25 | 1.32        | 1.52     |
| 3   | L     | 502 | D5M  | C2'-C1' | -7.25 | 1.32        | 1.52     |
| 3   | A     | 502 | D5M  | C2'-C1' | -7.24 | 1.32        | 1.52     |
| 3   | C     | 502 | D5M  | C2'-C1' | -7.24 | 1.32        | 1.52     |
| 3   | K     | 502 | D5M  | C2'-C1' | -7.23 | 1.32        | 1.52     |
| 3   | G     | 502 | D5M  | C2'-C1' | -7.21 | 1.32        | 1.52     |
| 2   | J     | 501 | DGT  | C4-N3   | 5.91  | 1.48        | 1.34     |
| 2   | H     | 501 | DGT  | C2-N3   | 5.90  | 1.47        | 1.33     |
| 2   | J     | 501 | DGT  | C2-N3   | 5.90  | 1.47        | 1.33     |
| 2   | H     | 501 | DGT  | C4-N3   | 5.90  | 1.48        | 1.34     |
| 2   | M     | 501 | DGT  | C2-N3   | 5.86  | 1.47        | 1.33     |
| 2   | L     | 501 | DGT  | C4-N3   | 5.86  | 1.48        | 1.34     |
| 2   | N     | 501 | DGT  | C2-N3   | 5.85  | 1.47        | 1.33     |
| 2   | A     | 501 | DGT  | C2-N3   | 5.85  | 1.47        | 1.33     |
| 2   | E     | 501 | DGT  | C2-N3   | 5.85  | 1.47        | 1.33     |
| 2   | C     | 501 | DGT  | C2-N3   | 5.85  | 1.47        | 1.33     |
| 2   | F     | 501 | DGT  | C2-N3   | 5.84  | 1.47        | 1.33     |
| 2   | G     | 501 | DGT  | C2-N3   | 5.83  | 1.47        | 1.33     |
| 2   | D     | 501 | DGT  | C2-N3   | 5.82  | 1.47        | 1.33     |
| 2   | K     | 501 | DGT  | C4-N3   | 5.82  | 1.48        | 1.34     |
| 2   | F     | 501 | DGT  | C4-N3   | 5.82  | 1.48        | 1.34     |
| 2   | D     | 501 | DGT  | C4-N3   | 5.82  | 1.48        | 1.34     |
| 2   | A     | 501 | DGT  | C4-N3   | 5.81  | 1.48        | 1.34     |
| 2   | E     | 501 | DGT  | C4-N3   | 5.81  | 1.48        | 1.34     |
| 3   | B     | 502 | D5M  | O4'-C4' | 5.80  | 1.58        | 1.45     |
| 2   | C     | 501 | DGT  | C4-N3   | 5.80  | 1.48        | 1.34     |
| 2   | M     | 501 | DGT  | C4-N3   | 5.80  | 1.48        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | P     | 501 | DGT  | C2-N3   | 5.80  | 1.47        | 1.33     |
| 2   | K     | 501 | DGT  | C2-N3   | 5.80  | 1.47        | 1.33     |
| 3   | D     | 502 | D5M  | O4'-C4' | 5.80  | 1.57        | 1.45     |
| 2   | N     | 501 | DGT  | C4-N3   | 5.79  | 1.48        | 1.34     |
| 2   | L     | 501 | DGT  | C2-N3   | 5.79  | 1.47        | 1.33     |
| 2   | I     | 501 | DGT  | C4-N3   | 5.79  | 1.48        | 1.34     |
| 3   | F     | 502 | D5M  | O4'-C4' | 5.78  | 1.57        | 1.45     |
| 2   | G     | 501 | DGT  | C4-N3   | 5.77  | 1.48        | 1.34     |
| 2   | P     | 501 | DGT  | C4-N3   | 5.76  | 1.48        | 1.34     |
| 2   | I     | 501 | DGT  | C2-N3   | 5.76  | 1.47        | 1.33     |
| 3   | N     | 502 | D5M  | O4'-C4' | 5.73  | 1.57        | 1.45     |
| 3   | P     | 502 | D5M  | O4'-C4' | 5.71  | 1.57        | 1.45     |
| 3   | C     | 502 | D5M  | O4'-C4' | 5.69  | 1.57        | 1.45     |
| 3   | J     | 502 | D5M  | O4'-C4' | 5.68  | 1.57        | 1.45     |
| 3   | G     | 502 | D5M  | O4'-C4' | 5.67  | 1.57        | 1.45     |
| 3   | A     | 502 | D5M  | O4'-C4' | 5.67  | 1.57        | 1.45     |
| 3   | I     | 502 | D5M  | O4'-C4' | 5.66  | 1.57        | 1.45     |
| 3   | E     | 502 | D5M  | O4'-C4' | 5.65  | 1.57        | 1.45     |
| 3   | M     | 502 | D5M  | O4'-C4' | 5.64  | 1.57        | 1.45     |
| 3   | H     | 502 | D5M  | O4'-C4' | 5.62  | 1.57        | 1.45     |
| 3   | L     | 502 | D5M  | O4'-C4' | 5.60  | 1.57        | 1.45     |
| 2   | B     | 501 | DGT  | C2-N3   | 5.59  | 1.46        | 1.33     |
| 3   | O     | 502 | D5M  | O4'-C4' | 5.58  | 1.57        | 1.45     |
| 2   | B     | 501 | DGT  | C4-N3   | 5.57  | 1.47        | 1.34     |
| 3   | K     | 502 | D5M  | O4'-C4' | 5.57  | 1.57        | 1.45     |
| 2   | O     | 501 | DGT  | C2-N3   | 5.56  | 1.46        | 1.33     |
| 2   | O     | 501 | DGT  | C4-N3   | 5.55  | 1.47        | 1.34     |
| 2   | J     | 501 | DGT  | O4'-C4' | 5.50  | 1.57        | 1.45     |
| 2   | C     | 501 | DGT  | O4'-C4' | 5.50  | 1.57        | 1.45     |
| 2   | K     | 501 | DGT  | O4'-C4' | 5.49  | 1.57        | 1.45     |
| 2   | H     | 501 | DGT  | O4'-C4' | 5.49  | 1.57        | 1.45     |
| 2   | A     | 501 | DGT  | O4'-C4' | 5.47  | 1.57        | 1.45     |
| 2   | F     | 501 | DGT  | O4'-C4' | 5.46  | 1.57        | 1.45     |
| 2   | D     | 501 | DGT  | O4'-C4' | 5.46  | 1.57        | 1.45     |
| 2   | N     | 501 | DGT  | O4'-C4' | 5.46  | 1.57        | 1.45     |
| 2   | E     | 501 | DGT  | O4'-C4' | 5.46  | 1.57        | 1.45     |
| 2   | L     | 501 | DGT  | O4'-C4' | 5.45  | 1.57        | 1.45     |
| 2   | G     | 501 | DGT  | O4'-C4' | 5.44  | 1.57        | 1.45     |
| 2   | M     | 501 | DGT  | O4'-C4' | 5.44  | 1.57        | 1.45     |
| 2   | I     | 501 | DGT  | O4'-C4' | 5.43  | 1.57        | 1.45     |
| 2   | P     | 501 | DGT  | O4'-C4' | 5.41  | 1.57        | 1.45     |
| 2   | P     | 501 | DGT  | O4'-C1' | -5.39 | 1.30        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | O     | 502 | D5M  | C6-N6   | 5.38  | 1.47        | 1.34     |
| 3   | A     | 502 | D5M  | C6-N6   | 5.38  | 1.47        | 1.34     |
| 3   | J     | 502 | D5M  | C6-N6   | 5.38  | 1.47        | 1.34     |
| 2   | G     | 501 | DGT  | O4'-C1' | -5.37 | 1.30        | 1.42     |
| 3   | B     | 502 | D5M  | C6-N6   | 5.37  | 1.47        | 1.34     |
| 3   | I     | 502 | D5M  | C6-N6   | 5.37  | 1.47        | 1.34     |
| 3   | G     | 502 | D5M  | C6-N6   | 5.36  | 1.47        | 1.34     |
| 3   | F     | 502 | D5M  | C6-N6   | 5.36  | 1.47        | 1.34     |
| 3   | E     | 502 | D5M  | C6-N6   | 5.36  | 1.47        | 1.34     |
| 2   | B     | 501 | DGT  | O4'-C4' | 5.36  | 1.57        | 1.45     |
| 3   | P     | 502 | D5M  | C6-N6   | 5.36  | 1.47        | 1.34     |
| 2   | O     | 501 | DGT  | O4'-C4' | 5.35  | 1.57        | 1.45     |
| 2   | F     | 501 | DGT  | O4'-C1' | -5.35 | 1.30        | 1.42     |
| 3   | D     | 502 | D5M  | C6-N6   | 5.35  | 1.47        | 1.34     |
| 2   | E     | 501 | DGT  | O4'-C1' | -5.35 | 1.30        | 1.42     |
| 3   | C     | 502 | D5M  | C6-N6   | 5.34  | 1.47        | 1.34     |
| 2   | M     | 501 | DGT  | O4'-C1' | -5.34 | 1.30        | 1.42     |
| 3   | H     | 502 | D5M  | C6-N6   | 5.34  | 1.47        | 1.34     |
| 3   | M     | 502 | D5M  | C6-N6   | 5.34  | 1.47        | 1.34     |
| 3   | N     | 502 | D5M  | C6-N6   | 5.33  | 1.47        | 1.34     |
| 2   | N     | 501 | DGT  | O4'-C1' | -5.32 | 1.30        | 1.42     |
| 3   | L     | 502 | D5M  | C6-N6   | 5.30  | 1.47        | 1.34     |
| 2   | C     | 501 | DGT  | O4'-C1' | -5.30 | 1.30        | 1.42     |
| 2   | A     | 501 | DGT  | O4'-C1' | -5.30 | 1.30        | 1.42     |
| 2   | D     | 501 | DGT  | O4'-C1' | -5.28 | 1.30        | 1.42     |
| 2   | I     | 501 | DGT  | O4'-C1' | -5.26 | 1.30        | 1.42     |
| 3   | K     | 502 | D5M  | C6-N6   | 5.25  | 1.47        | 1.34     |
| 2   | K     | 501 | DGT  | O4'-C1' | -5.22 | 1.30        | 1.42     |
| 2   | L     | 501 | DGT  | O4'-C1' | -5.21 | 1.30        | 1.42     |
| 2   | J     | 501 | DGT  | O4'-C1' | -5.17 | 1.30        | 1.42     |
| 2   | H     | 501 | DGT  | O4'-C1' | -5.16 | 1.30        | 1.42     |
| 2   | O     | 501 | DGT  | O4'-C1' | -5.07 | 1.31        | 1.42     |
| 2   | B     | 501 | DGT  | O4'-C1' | -5.04 | 1.31        | 1.42     |
| 3   | K     | 502 | D5M  | O4'-C1' | 4.81  | 1.53        | 1.42     |
| 3   | L     | 502 | D5M  | O4'-C1' | 4.77  | 1.53        | 1.42     |
| 3   | A     | 502 | D5M  | O4'-C1' | 4.75  | 1.53        | 1.42     |
| 3   | P     | 502 | D5M  | O4'-C1' | 4.74  | 1.52        | 1.42     |
| 3   | J     | 502 | D5M  | O4'-C1' | 4.73  | 1.52        | 1.42     |
| 3   | G     | 502 | D5M  | O4'-C1' | 4.73  | 1.52        | 1.42     |
| 3   | N     | 502 | D5M  | O4'-C1' | 4.73  | 1.52        | 1.42     |
| 3   | M     | 502 | D5M  | O4'-C1' | 4.72  | 1.52        | 1.42     |
| 3   | C     | 502 | D5M  | O4'-C1' | 4.70  | 1.52        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | E     | 502 | D5M  | O4'-C1' | 4.68  | 1.52        | 1.42     |
| 3   | I     | 502 | D5M  | O4'-C1' | 4.68  | 1.52        | 1.42     |
| 3   | O     | 502 | D5M  | O4'-C1' | 4.66  | 1.52        | 1.42     |
| 3   | H     | 502 | D5M  | O4'-C1' | 4.64  | 1.52        | 1.42     |
| 3   | D     | 502 | D5M  | O4'-C1' | 4.63  | 1.52        | 1.42     |
| 3   | B     | 502 | D5M  | O4'-C1' | 4.63  | 1.52        | 1.42     |
| 3   | F     | 502 | D5M  | O4'-C1' | 4.58  | 1.52        | 1.42     |
| 2   | H     | 501 | DGT  | C2-N2   | 4.53  | 1.45        | 1.34     |
| 2   | P     | 501 | DGT  | C2-N2   | 4.52  | 1.44        | 1.34     |
| 2   | J     | 501 | DGT  | C2-N2   | 4.51  | 1.44        | 1.34     |
| 2   | N     | 501 | DGT  | C2-N2   | 4.51  | 1.44        | 1.34     |
| 2   | C     | 501 | DGT  | C2-N2   | 4.50  | 1.44        | 1.34     |
| 2   | L     | 501 | DGT  | C2-N2   | 4.49  | 1.44        | 1.34     |
| 2   | F     | 501 | DGT  | C2-N2   | 4.49  | 1.44        | 1.34     |
| 2   | A     | 501 | DGT  | C2-N2   | 4.48  | 1.44        | 1.34     |
| 2   | D     | 501 | DGT  | C2-N2   | 4.47  | 1.44        | 1.34     |
| 2   | G     | 501 | DGT  | C2-N2   | 4.47  | 1.44        | 1.34     |
| 2   | B     | 501 | DGT  | C5'-C4' | -4.47 | 1.37        | 1.51     |
| 2   | E     | 501 | DGT  | C2-N2   | 4.46  | 1.44        | 1.34     |
| 2   | M     | 501 | DGT  | C2-N2   | 4.46  | 1.44        | 1.34     |
| 2   | I     | 501 | DGT  | C2-N2   | 4.46  | 1.44        | 1.34     |
| 2   | O     | 501 | DGT  | C5'-C4' | -4.45 | 1.37        | 1.51     |
| 2   | K     | 501 | DGT  | C2-N2   | 4.44  | 1.44        | 1.34     |
| 2   | I     | 501 | DGT  | C5'-C4' | -4.44 | 1.37        | 1.51     |
| 2   | D     | 501 | DGT  | C5'-C4' | -4.41 | 1.37        | 1.51     |
| 2   | L     | 501 | DGT  | C5'-C4' | -4.41 | 1.37        | 1.51     |
| 2   | G     | 501 | DGT  | C5'-C4' | -4.37 | 1.38        | 1.51     |
| 2   | J     | 501 | DGT  | C5'-C4' | -4.36 | 1.38        | 1.51     |
| 2   | H     | 501 | DGT  | C5'-C4' | -4.36 | 1.38        | 1.51     |
| 2   | P     | 501 | DGT  | C5'-C4' | -4.33 | 1.38        | 1.51     |
| 2   | K     | 501 | DGT  | C5'-C4' | -4.32 | 1.38        | 1.51     |
| 2   | F     | 501 | DGT  | C5'-C4' | -4.31 | 1.38        | 1.51     |
| 2   | H     | 501 | DGT  | C2'-C1' | 4.31  | 1.64        | 1.52     |
| 3   | C     | 502 | D5M  | C2'-C3' | 4.30  | 1.64        | 1.52     |
| 2   | E     | 501 | DGT  | C5'-C4' | -4.30 | 1.38        | 1.51     |
| 2   | A     | 501 | DGT  | C5'-C4' | -4.30 | 1.38        | 1.51     |
| 2   | M     | 501 | DGT  | C5'-C4' | -4.29 | 1.38        | 1.51     |
| 2   | N     | 501 | DGT  | C5'-C4' | -4.29 | 1.38        | 1.51     |
| 2   | C     | 501 | DGT  | C5'-C4' | -4.28 | 1.38        | 1.51     |
| 2   | J     | 501 | DGT  | C2'-C1' | 4.28  | 1.64        | 1.52     |
| 3   | O     | 502 | D5M  | C2'-C3' | 4.27  | 1.64        | 1.52     |
| 3   | H     | 502 | D5M  | C2'-C3' | 4.25  | 1.64        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | F     | 502 | D5M  | C2'-C3' | 4.24  | 1.64        | 1.52     |
| 3   | K     | 502 | D5M  | C2'-C3' | 4.24  | 1.64        | 1.52     |
| 3   | E     | 502 | D5M  | C2'-C3' | 4.24  | 1.64        | 1.52     |
| 3   | D     | 502 | D5M  | C2'-C3' | 4.24  | 1.64        | 1.52     |
| 2   | B     | 501 | DGT  | C2-N2   | 4.21  | 1.44        | 1.34     |
| 2   | O     | 501 | DGT  | C2-N2   | 4.20  | 1.44        | 1.34     |
| 3   | M     | 502 | D5M  | C2'-C3' | 4.20  | 1.64        | 1.52     |
| 3   | B     | 502 | D5M  | C2'-C3' | 4.19  | 1.64        | 1.52     |
| 3   | A     | 502 | D5M  | C2'-C3' | 4.18  | 1.63        | 1.52     |
| 2   | O     | 501 | DGT  | C2'-C1' | 4.18  | 1.64        | 1.52     |
| 3   | G     | 502 | D5M  | C2'-C3' | 4.18  | 1.63        | 1.52     |
| 3   | I     | 502 | D5M  | C2'-C3' | 4.17  | 1.63        | 1.52     |
| 3   | L     | 502 | D5M  | C2'-C3' | 4.17  | 1.63        | 1.52     |
| 2   | D     | 501 | DGT  | C2'-C1' | 4.16  | 1.64        | 1.52     |
| 2   | B     | 501 | DGT  | C2'-C1' | 4.16  | 1.64        | 1.52     |
| 2   | E     | 501 | DGT  | C2'-C1' | 4.16  | 1.64        | 1.52     |
| 3   | J     | 502 | D5M  | C2'-C3' | 4.16  | 1.63        | 1.52     |
| 2   | A     | 501 | DGT  | C2'-C1' | 4.16  | 1.64        | 1.52     |
| 2   | F     | 501 | DGT  | C2'-C1' | 4.15  | 1.64        | 1.52     |
| 2   | M     | 501 | DGT  | C2'-C1' | 4.15  | 1.63        | 1.52     |
| 2   | N     | 501 | DGT  | C2'-C1' | 4.14  | 1.63        | 1.52     |
| 2   | P     | 501 | DGT  | C2'-C1' | 4.12  | 1.63        | 1.52     |
| 3   | N     | 502 | D5M  | C2'-C3' | 4.11  | 1.63        | 1.52     |
| 2   | C     | 501 | DGT  | C2'-C1' | 4.11  | 1.63        | 1.52     |
| 2   | K     | 501 | DGT  | C2'-C1' | 4.09  | 1.63        | 1.52     |
| 3   | P     | 502 | D5M  | C2'-C3' | 4.09  | 1.63        | 1.52     |
| 2   | L     | 501 | DGT  | C2'-C1' | 4.09  | 1.63        | 1.52     |
| 2   | G     | 501 | DGT  | C2'-C1' | 4.09  | 1.63        | 1.52     |
| 2   | I     | 501 | DGT  | C2'-C1' | 4.07  | 1.63        | 1.52     |
| 2   | J     | 501 | DGT  | C5-N7   | -3.08 | 1.33        | 1.39     |
| 2   | A     | 501 | DGT  | C5-N7   | -3.07 | 1.33        | 1.39     |
| 2   | F     | 501 | DGT  | C5-N7   | -3.07 | 1.33        | 1.39     |
| 2   | O     | 501 | DGT  | C5-N7   | -3.07 | 1.33        | 1.39     |
| 2   | M     | 501 | DGT  | C5-N7   | -3.07 | 1.33        | 1.39     |
| 2   | E     | 501 | DGT  | C5-N7   | -3.06 | 1.33        | 1.39     |
| 2   | B     | 501 | DGT  | C5-N7   | -3.06 | 1.33        | 1.39     |
| 2   | K     | 501 | DGT  | C5-N7   | -3.06 | 1.33        | 1.39     |
| 2   | D     | 501 | DGT  | C5-N7   | -3.06 | 1.33        | 1.39     |
| 2   | N     | 501 | DGT  | C5-N7   | -3.05 | 1.33        | 1.39     |
| 2   | I     | 501 | DGT  | C5-N7   | -3.05 | 1.33        | 1.39     |
| 2   | C     | 501 | DGT  | C5-N7   | -3.05 | 1.33        | 1.39     |
| 2   | G     | 501 | DGT  | C5-N7   | -3.04 | 1.33        | 1.39     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | H     | 501 | DGT  | C5-N7 | -3.04 | 1.33        | 1.39     |
| 2   | L     | 501 | DGT  | C5-N7 | -3.03 | 1.33        | 1.39     |
| 2   | P     | 501 | DGT  | C5-N7 | -3.00 | 1.33        | 1.39     |
| 3   | K     | 502 | D5M  | C5-C4 | -2.94 | 1.33        | 1.39     |
| 3   | L     | 502 | D5M  | C5-C4 | -2.89 | 1.33        | 1.39     |
| 3   | I     | 502 | D5M  | C5-C4 | -2.87 | 1.33        | 1.39     |
| 2   | P     | 501 | DGT  | C2-N1 | 2.87  | 1.44        | 1.37     |
| 2   | A     | 501 | DGT  | C2-N1 | 2.86  | 1.44        | 1.37     |
| 2   | C     | 501 | DGT  | C2-N1 | 2.85  | 1.44        | 1.37     |
| 2   | D     | 501 | DGT  | C2-N1 | 2.85  | 1.44        | 1.37     |
| 2   | F     | 501 | DGT  | C2-N1 | 2.85  | 1.44        | 1.37     |
| 3   | L     | 502 | D5M  | C5-N7 | -2.85 | 1.33        | 1.39     |
| 2   | O     | 501 | DGT  | C2-N1 | 2.85  | 1.44        | 1.37     |
| 2   | G     | 501 | DGT  | C2-N1 | 2.85  | 1.44        | 1.37     |
| 2   | E     | 501 | DGT  | C2-N1 | 2.85  | 1.44        | 1.37     |
| 2   | I     | 501 | DGT  | C2-N1 | 2.84  | 1.44        | 1.37     |
| 2   | B     | 501 | DGT  | C2-N1 | 2.84  | 1.44        | 1.37     |
| 3   | H     | 502 | D5M  | C5-N7 | -2.84 | 1.33        | 1.39     |
| 3   | B     | 502 | D5M  | C5-C4 | -2.84 | 1.33        | 1.39     |
| 3   | O     | 502 | D5M  | C5-C4 | -2.84 | 1.33        | 1.39     |
| 3   | N     | 502 | D5M  | C5-C4 | -2.84 | 1.33        | 1.39     |
| 2   | J     | 501 | DGT  | C2-N1 | 2.84  | 1.44        | 1.37     |
| 2   | N     | 501 | DGT  | C2-N1 | 2.84  | 1.44        | 1.37     |
| 2   | M     | 501 | DGT  | C2-N1 | 2.84  | 1.44        | 1.37     |
| 3   | D     | 502 | D5M  | C5-C4 | -2.83 | 1.33        | 1.39     |
| 2   | L     | 501 | DGT  | C2-N1 | 2.83  | 1.44        | 1.37     |
| 3   | J     | 502 | D5M  | C5-C4 | -2.82 | 1.33        | 1.39     |
| 3   | M     | 502 | D5M  | C5-C4 | -2.81 | 1.33        | 1.39     |
| 2   | H     | 501 | DGT  | C2-N1 | 2.81  | 1.44        | 1.37     |
| 2   | K     | 501 | DGT  | C2-N1 | 2.81  | 1.44        | 1.37     |
| 3   | E     | 502 | D5M  | C5-C4 | -2.81 | 1.33        | 1.39     |
| 2   | M     | 501 | DGT  | C5-C6 | 2.81  | 1.54        | 1.44     |
| 3   | K     | 502 | D5M  | C5-N7 | -2.81 | 1.33        | 1.39     |
| 3   | H     | 502 | D5M  | C5-C4 | -2.81 | 1.33        | 1.39     |
| 3   | B     | 502 | D5M  | C5-N7 | -2.80 | 1.33        | 1.39     |
| 3   | J     | 502 | D5M  | C5-N7 | -2.80 | 1.33        | 1.39     |
| 2   | E     | 501 | DGT  | C5-C6 | 2.80  | 1.54        | 1.44     |
| 3   | E     | 502 | D5M  | C5-N7 | -2.80 | 1.33        | 1.39     |
| 3   | F     | 502 | D5M  | C5-N7 | -2.80 | 1.33        | 1.39     |
| 3   | A     | 502 | D5M  | C5-C4 | -2.79 | 1.33        | 1.39     |
| 3   | P     | 502 | D5M  | C5-C4 | -2.79 | 1.33        | 1.39     |
| 2   | D     | 501 | DGT  | C5-C6 | 2.79  | 1.54        | 1.44     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | F     | 501 | DGT  | C5-C6  | 2.79  | 1.54        | 1.44     |
| 2   | N     | 501 | DGT  | C5-C6  | 2.79  | 1.54        | 1.44     |
| 3   | G     | 502 | D5M  | C5-C4  | -2.79 | 1.33        | 1.39     |
| 2   | O     | 501 | DGT  | C5-C6  | 2.79  | 1.54        | 1.44     |
| 3   | C     | 502 | D5M  | C5-N7  | -2.78 | 1.33        | 1.39     |
| 3   | F     | 502 | D5M  | C5-C4  | -2.78 | 1.33        | 1.39     |
| 2   | A     | 501 | DGT  | C5-C6  | 2.78  | 1.54        | 1.44     |
| 3   | N     | 502 | D5M  | C5-N7  | -2.78 | 1.33        | 1.39     |
| 2   | B     | 501 | DGT  | C5-C6  | 2.78  | 1.54        | 1.44     |
| 3   | A     | 502 | D5M  | C5-N7  | -2.78 | 1.33        | 1.39     |
| 3   | M     | 502 | D5M  | C5-N7  | -2.78 | 1.33        | 1.39     |
| 3   | G     | 502 | D5M  | C5-N7  | -2.77 | 1.33        | 1.39     |
| 2   | P     | 501 | DGT  | C5-C6  | 2.77  | 1.54        | 1.44     |
| 3   | O     | 502 | D5M  | C5-N7  | -2.77 | 1.33        | 1.39     |
| 3   | I     | 502 | D5M  | C5-N7  | -2.77 | 1.33        | 1.39     |
| 2   | K     | 501 | DGT  | C5-C6  | 2.77  | 1.54        | 1.44     |
| 3   | C     | 502 | D5M  | C5-C4  | -2.77 | 1.33        | 1.39     |
| 3   | P     | 502 | D5M  | C5-N7  | -2.77 | 1.33        | 1.39     |
| 2   | C     | 501 | DGT  | C5-C6  | 2.76  | 1.54        | 1.44     |
| 2   | G     | 501 | DGT  | C5-C6  | 2.76  | 1.54        | 1.44     |
| 2   | J     | 501 | DGT  | C5-C6  | 2.75  | 1.54        | 1.44     |
| 2   | I     | 501 | DGT  | C5-C6  | 2.75  | 1.54        | 1.44     |
| 2   | H     | 501 | DGT  | C5-C6  | 2.74  | 1.54        | 1.44     |
| 2   | L     | 501 | DGT  | C5-C6  | 2.74  | 1.54        | 1.44     |
| 3   | D     | 502 | D5M  | C5-N7  | -2.73 | 1.33        | 1.39     |
| 2   | F     | 501 | DGT  | PG-O3G | 2.61  | 1.58        | 1.50     |
| 2   | J     | 501 | DGT  | PG-O3G | 2.60  | 1.58        | 1.50     |
| 2   | G     | 501 | DGT  | PG-O3G | 2.59  | 1.58        | 1.50     |
| 2   | A     | 501 | DGT  | PG-O3G | 2.58  | 1.58        | 1.50     |
| 2   | L     | 501 | DGT  | PG-O3G | 2.58  | 1.58        | 1.50     |
| 2   | E     | 501 | DGT  | PG-O3G | 2.58  | 1.58        | 1.50     |
| 2   | D     | 501 | DGT  | PG-O3G | 2.58  | 1.58        | 1.50     |
| 2   | H     | 501 | DGT  | PG-O3G | 2.57  | 1.58        | 1.50     |
| 2   | M     | 501 | DGT  | PG-O3G | 2.57  | 1.58        | 1.50     |
| 2   | N     | 501 | DGT  | PG-O3G | 2.57  | 1.58        | 1.50     |
| 2   | P     | 501 | DGT  | PG-O3G | 2.56  | 1.58        | 1.50     |
| 2   | O     | 501 | DGT  | PG-O3G | 2.56  | 1.58        | 1.50     |
| 3   | O     | 502 | D5M  | C4-N9  | -2.56 | 1.32        | 1.37     |
| 2   | I     | 501 | DGT  | PG-O3G | 2.55  | 1.58        | 1.50     |
| 2   | K     | 501 | DGT  | PG-O3G | 2.55  | 1.58        | 1.50     |
| 3   | N     | 502 | D5M  | C4-N9  | -2.54 | 1.32        | 1.37     |
| 2   | B     | 501 | DGT  | PG-O3G | 2.54  | 1.58        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | C     | 501 | DGT  | PG-O3G  | 2.53  | 1.58        | 1.50     |
| 3   | M     | 502 | D5M  | C4-N9   | -2.52 | 1.32        | 1.37     |
| 3   | P     | 502 | D5M  | C4-N9   | -2.52 | 1.32        | 1.37     |
| 3   | J     | 502 | D5M  | C4-N9   | -2.51 | 1.32        | 1.37     |
| 3   | B     | 502 | D5M  | C4-N9   | -2.51 | 1.32        | 1.37     |
| 3   | I     | 502 | D5M  | C4-N9   | -2.51 | 1.32        | 1.37     |
| 3   | G     | 502 | D5M  | C4-N9   | -2.50 | 1.32        | 1.37     |
| 3   | A     | 502 | D5M  | C4-N9   | -2.50 | 1.32        | 1.37     |
| 3   | H     | 502 | D5M  | C4-N9   | -2.49 | 1.32        | 1.37     |
| 3   | E     | 502 | D5M  | C4-N9   | -2.47 | 1.32        | 1.37     |
| 3   | L     | 502 | D5M  | C4-N9   | -2.47 | 1.32        | 1.37     |
| 3   | D     | 502 | D5M  | C4-N9   | -2.47 | 1.32        | 1.37     |
| 3   | C     | 502 | D5M  | C4-N9   | -2.46 | 1.32        | 1.37     |
| 3   | F     | 502 | D5M  | C4-N9   | -2.45 | 1.32        | 1.37     |
| 3   | K     | 502 | D5M  | C4-N9   | -2.42 | 1.32        | 1.37     |
| 2   | G     | 501 | DGT  | O3'-C3' | 2.33  | 1.48        | 1.43     |
| 2   | C     | 501 | DGT  | O3'-C3' | 2.32  | 1.48        | 1.43     |
| 2   | F     | 501 | DGT  | O3'-C3' | 2.30  | 1.48        | 1.43     |
| 2   | A     | 501 | DGT  | O3'-C3' | 2.30  | 1.48        | 1.43     |
| 2   | H     | 501 | DGT  | O3'-C3' | 2.30  | 1.48        | 1.43     |
| 2   | E     | 501 | DGT  | O3'-C3' | 2.30  | 1.48        | 1.43     |
| 2   | P     | 501 | DGT  | O3'-C3' | 2.29  | 1.48        | 1.43     |
| 2   | N     | 501 | DGT  | O3'-C3' | 2.28  | 1.48        | 1.43     |
| 2   | M     | 501 | DGT  | O3'-C3' | 2.28  | 1.48        | 1.43     |
| 2   | B     | 501 | DGT  | O3'-C3' | 2.27  | 1.48        | 1.43     |
| 2   | K     | 501 | DGT  | O3'-C3' | 2.27  | 1.48        | 1.43     |
| 2   | O     | 501 | DGT  | O3'-C3' | 2.27  | 1.48        | 1.43     |
| 2   | L     | 501 | DGT  | O3'-C3' | 2.27  | 1.48        | 1.43     |
| 2   | I     | 501 | DGT  | O3'-C3' | 2.27  | 1.48        | 1.43     |
| 2   | D     | 501 | DGT  | O3'-C3' | 2.26  | 1.48        | 1.43     |
| 2   | J     | 501 | DGT  | O3'-C3' | 2.26  | 1.48        | 1.43     |
| 2   | A     | 501 | DGT  | PA-O5'  | 2.23  | 1.68        | 1.59     |
| 2   | F     | 501 | DGT  | PA-O5'  | 2.22  | 1.68        | 1.59     |
| 2   | N     | 501 | DGT  | PA-O5'  | 2.21  | 1.68        | 1.59     |
| 2   | E     | 501 | DGT  | PA-O5'  | 2.21  | 1.68        | 1.59     |
| 2   | C     | 501 | DGT  | PA-O5'  | 2.21  | 1.68        | 1.59     |
| 2   | K     | 501 | DGT  | PA-O5'  | 2.21  | 1.68        | 1.59     |
| 2   | M     | 501 | DGT  | PA-O5'  | 2.20  | 1.68        | 1.59     |
| 2   | F     | 501 | DGT  | PG-O2G  | -2.20 | 1.46        | 1.54     |
| 2   | A     | 501 | DGT  | PG-O2G  | -2.19 | 1.46        | 1.54     |
| 2   | K     | 501 | DGT  | PG-O2G  | -2.19 | 1.46        | 1.54     |
| 2   | E     | 501 | DGT  | PG-O2G  | -2.19 | 1.46        | 1.54     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | J     | 501 | DGT  | PG-O2G | -2.19 | 1.46        | 1.54     |
| 2   | P     | 501 | DGT  | PG-O2G | -2.18 | 1.46        | 1.54     |
| 2   | G     | 501 | DGT  | PA-O5' | 2.18  | 1.68        | 1.59     |
| 2   | B     | 501 | DGT  | PG-O2G | -2.18 | 1.46        | 1.54     |
| 2   | L     | 501 | DGT  | PG-O2G | -2.18 | 1.46        | 1.54     |
| 2   | P     | 501 | DGT  | PA-O5' | 2.18  | 1.68        | 1.59     |
| 2   | M     | 501 | DGT  | PG-O2G | -2.18 | 1.46        | 1.54     |
| 2   | O     | 501 | DGT  | PG-O2G | -2.18 | 1.46        | 1.54     |
| 2   | I     | 501 | DGT  | PG-O2G | -2.18 | 1.46        | 1.54     |
| 2   | N     | 501 | DGT  | PG-O2G | -2.18 | 1.46        | 1.54     |
| 2   | H     | 501 | DGT  | PA-O5' | 2.17  | 1.68        | 1.59     |
| 2   | H     | 501 | DGT  | PG-O2G | -2.17 | 1.46        | 1.54     |
| 2   | J     | 501 | DGT  | PA-O5' | 2.17  | 1.68        | 1.59     |
| 2   | G     | 501 | DGT  | PG-O2G | -2.16 | 1.46        | 1.54     |
| 2   | L     | 501 | DGT  | PA-O5' | 2.16  | 1.68        | 1.59     |
| 2   | D     | 501 | DGT  | PG-O2G | -2.16 | 1.46        | 1.54     |
| 2   | D     | 501 | DGT  | PA-O5' | 2.15  | 1.68        | 1.59     |
| 2   | I     | 501 | DGT  | PA-O5' | 2.15  | 1.68        | 1.59     |
| 2   | C     | 501 | DGT  | PG-O2G | -2.14 | 1.46        | 1.54     |
| 2   | B     | 501 | DGT  | PA-O5' | 2.07  | 1.67        | 1.59     |
| 2   | O     | 501 | DGT  | PA-O5' | 2.06  | 1.67        | 1.59     |
| 2   | H     | 501 | DGT  | C8-N9  | -2.02 | 1.33        | 1.37     |
| 2   | J     | 501 | DGT  | C8-N9  | -2.00 | 1.33        | 1.37     |

All (399) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | N     | 501 | DGT  | C1'-N9-C8 | -8.72 | 108.29      | 127.85   |
| 2   | M     | 501 | DGT  | C1'-N9-C8 | -8.72 | 108.31      | 127.85   |
| 2   | E     | 501 | DGT  | C1'-N9-C8 | -8.71 | 108.33      | 127.85   |
| 2   | C     | 501 | DGT  | C1'-N9-C8 | -8.70 | 108.35      | 127.85   |
| 2   | F     | 501 | DGT  | C1'-N9-C8 | -8.70 | 108.36      | 127.85   |
| 2   | A     | 501 | DGT  | C1'-N9-C8 | -8.69 | 108.37      | 127.85   |
| 2   | L     | 501 | DGT  | C1'-N9-C8 | -8.69 | 108.37      | 127.85   |
| 2   | K     | 501 | DGT  | C1'-N9-C8 | -8.68 | 108.41      | 127.85   |
| 2   | J     | 501 | DGT  | C1'-N9-C8 | -8.66 | 108.45      | 127.85   |
| 2   | P     | 501 | DGT  | C1'-N9-C8 | -8.65 | 108.47      | 127.85   |
| 2   | I     | 501 | DGT  | C1'-N9-C8 | -8.64 | 108.47      | 127.85   |
| 2   | H     | 501 | DGT  | C1'-N9-C8 | -8.64 | 108.48      | 127.85   |
| 2   | D     | 501 | DGT  | C1'-N9-C8 | -8.55 | 108.69      | 127.85   |
| 2   | G     | 501 | DGT  | C1'-N9-C8 | -8.45 | 108.91      | 127.85   |
| 2   | O     | 501 | DGT  | C1'-N9-C8 | -8.07 | 109.76      | 127.85   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | B     | 501 | DGT  | C1'-N9-C8 | -8.07 | 109.77      | 127.85   |
| 3   | L     | 502 | D5M  | N6-C6-N1  | -5.98 | 105.25      | 118.35   |
| 3   | D     | 502 | D5M  | N6-C6-N1  | -5.97 | 105.28      | 118.35   |
| 3   | A     | 502 | D5M  | N6-C6-N1  | -5.96 | 105.30      | 118.35   |
| 3   | O     | 502 | D5M  | N6-C6-N1  | -5.94 | 105.33      | 118.35   |
| 3   | C     | 502 | D5M  | N6-C6-N1  | -5.94 | 105.35      | 118.35   |
| 3   | P     | 502 | D5M  | N6-C6-N1  | -5.93 | 105.36      | 118.35   |
| 3   | F     | 502 | D5M  | N6-C6-N1  | -5.93 | 105.36      | 118.35   |
| 3   | M     | 502 | D5M  | N6-C6-N1  | -5.93 | 105.36      | 118.35   |
| 3   | G     | 502 | D5M  | N6-C6-N1  | -5.92 | 105.38      | 118.35   |
| 3   | H     | 502 | D5M  | N6-C6-N1  | -5.90 | 105.43      | 118.35   |
| 3   | I     | 502 | D5M  | N6-C6-N1  | -5.90 | 105.44      | 118.35   |
| 3   | J     | 502 | D5M  | N6-C6-N1  | -5.89 | 105.46      | 118.35   |
| 3   | E     | 502 | D5M  | N6-C6-N1  | -5.88 | 105.46      | 118.35   |
| 3   | K     | 502 | D5M  | N6-C6-N1  | -5.88 | 105.48      | 118.35   |
| 3   | B     | 502 | D5M  | N6-C6-N1  | -5.87 | 105.50      | 118.35   |
| 3   | N     | 502 | D5M  | N6-C6-N1  | -5.83 | 105.59      | 118.35   |
| 2   | N     | 501 | DGT  | C1'-N9-C4 | 5.68  | 141.22      | 125.48   |
| 2   | E     | 501 | DGT  | C1'-N9-C4 | 5.66  | 141.19      | 125.48   |
| 2   | M     | 501 | DGT  | C1'-N9-C4 | 5.66  | 141.19      | 125.48   |
| 2   | C     | 501 | DGT  | C1'-N9-C4 | 5.66  | 141.18      | 125.48   |
| 2   | F     | 501 | DGT  | C1'-N9-C4 | 5.66  | 141.18      | 125.48   |
| 2   | A     | 501 | DGT  | C1'-N9-C4 | 5.66  | 141.17      | 125.48   |
| 2   | K     | 501 | DGT  | C1'-N9-C4 | 5.64  | 141.12      | 125.48   |
| 2   | J     | 501 | DGT  | C1'-N9-C4 | 5.63  | 141.10      | 125.48   |
| 2   | H     | 501 | DGT  | C1'-N9-C4 | 5.63  | 141.09      | 125.48   |
| 2   | L     | 501 | DGT  | C1'-N9-C4 | 5.63  | 141.08      | 125.48   |
| 2   | I     | 501 | DGT  | C1'-N9-C4 | 5.58  | 140.94      | 125.48   |
| 2   | D     | 501 | DGT  | C1'-N9-C4 | 5.55  | 140.87      | 125.48   |
| 2   | P     | 501 | DGT  | C1'-N9-C4 | 5.55  | 140.86      | 125.48   |
| 3   | M     | 502 | D5M  | N3-C2-N1  | -5.52 | 119.96      | 128.60   |
| 3   | P     | 502 | D5M  | N3-C2-N1  | -5.50 | 120.00      | 128.60   |
| 3   | D     | 502 | D5M  | N3-C2-N1  | -5.50 | 120.00      | 128.60   |
| 3   | J     | 502 | D5M  | N3-C2-N1  | -5.49 | 120.02      | 128.60   |
| 3   | G     | 502 | D5M  | N3-C2-N1  | -5.48 | 120.03      | 128.60   |
| 3   | F     | 502 | D5M  | N3-C2-N1  | -5.48 | 120.03      | 128.60   |
| 3   | N     | 502 | D5M  | N3-C2-N1  | -5.47 | 120.05      | 128.60   |
| 3   | A     | 502 | D5M  | N3-C2-N1  | -5.45 | 120.07      | 128.60   |
| 3   | B     | 502 | D5M  | N3-C2-N1  | -5.45 | 120.08      | 128.60   |
| 3   | E     | 502 | D5M  | N3-C2-N1  | -5.44 | 120.09      | 128.60   |
| 3   | H     | 502 | D5M  | N3-C2-N1  | -5.43 | 120.10      | 128.60   |
| 3   | C     | 502 | D5M  | N3-C2-N1  | -5.43 | 120.11      | 128.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3   | K     | 502 | D5M  | C5-C4-N3  | -5.42 | 119.68      | 126.75   |
| 2   | G     | 501 | DGT  | C1'-N9-C4 | 5.41  | 140.47      | 125.48   |
| 3   | I     | 502 | D5M  | N3-C2-N1  | -5.40 | 120.15      | 128.60   |
| 3   | O     | 502 | D5M  | N3-C2-N1  | -5.39 | 120.18      | 128.60   |
| 3   | L     | 502 | D5M  | N3-C2-N1  | -5.38 | 120.19      | 128.60   |
| 3   | K     | 502 | D5M  | N3-C2-N1  | -5.27 | 120.36      | 128.60   |
| 3   | F     | 502 | D5M  | C5-C4-N3  | -5.26 | 119.89      | 126.75   |
| 3   | L     | 502 | D5M  | C5-C4-N3  | -5.24 | 119.92      | 126.75   |
| 3   | H     | 502 | D5M  | C5-C4-N3  | -5.23 | 119.92      | 126.75   |
| 2   | O     | 501 | DGT  | C1'-N9-C4 | 5.23  | 139.98      | 125.48   |
| 3   | E     | 502 | D5M  | C5-C4-N3  | -5.22 | 119.93      | 126.75   |
| 2   | B     | 501 | DGT  | C1'-N9-C4 | 5.22  | 139.96      | 125.48   |
| 3   | N     | 502 | D5M  | C5-C4-N3  | -5.22 | 119.94      | 126.75   |
| 3   | C     | 502 | D5M  | C5-C4-N3  | -5.22 | 119.95      | 126.75   |
| 3   | D     | 502 | D5M  | C5-C4-N3  | -5.21 | 119.96      | 126.75   |
| 3   | J     | 502 | D5M  | C5-C4-N3  | -5.20 | 119.97      | 126.75   |
| 3   | O     | 502 | D5M  | C5-C4-N3  | -5.20 | 119.97      | 126.75   |
| 3   | G     | 502 | D5M  | C5-C4-N3  | -5.18 | 119.99      | 126.75   |
| 3   | A     | 502 | D5M  | C5-C4-N3  | -5.18 | 120.00      | 126.75   |
| 3   | M     | 502 | D5M  | C5-C4-N3  | -5.18 | 120.00      | 126.75   |
| 3   | P     | 502 | D5M  | C5-C4-N3  | -5.16 | 120.01      | 126.75   |
| 3   | B     | 502 | D5M  | C5-C4-N3  | -5.16 | 120.02      | 126.75   |
| 3   | I     | 502 | D5M  | C5-C4-N3  | -5.15 | 120.03      | 126.75   |
| 3   | D     | 502 | D5M  | C5-C6-N6  | 5.11  | 134.56      | 123.43   |
| 3   | A     | 502 | D5M  | C5-C6-N6  | 5.09  | 134.51      | 123.43   |
| 3   | L     | 502 | D5M  | C5-C6-N6  | 5.08  | 134.49      | 123.43   |
| 3   | G     | 502 | D5M  | C5-C6-N6  | 5.08  | 134.48      | 123.43   |
| 3   | C     | 502 | D5M  | C5-C6-N6  | 5.07  | 134.47      | 123.43   |
| 3   | M     | 502 | D5M  | C5-C6-N6  | 5.07  | 134.47      | 123.43   |
| 3   | P     | 502 | D5M  | C5-C6-N6  | 5.07  | 134.46      | 123.43   |
| 3   | I     | 502 | D5M  | C5-C6-N6  | 5.06  | 134.44      | 123.43   |
| 3   | F     | 502 | D5M  | C5-C6-N6  | 5.06  | 134.43      | 123.43   |
| 3   | O     | 502 | D5M  | C5-C6-N6  | 5.05  | 134.41      | 123.43   |
| 3   | J     | 502 | D5M  | C5-C6-N6  | 5.04  | 134.40      | 123.43   |
| 3   | E     | 502 | D5M  | C5-C6-N6  | 5.03  | 134.39      | 123.43   |
| 3   | B     | 502 | D5M  | C5-C6-N6  | 5.02  | 134.36      | 123.43   |
| 3   | K     | 502 | D5M  | C5-C6-N6  | 5.02  | 134.36      | 123.43   |
| 3   | H     | 502 | D5M  | C5-C6-N6  | 5.02  | 134.35      | 123.43   |
| 3   | N     | 502 | D5M  | C5-C6-N6  | 4.99  | 134.29      | 123.43   |
| 2   | H     | 501 | DGT  | C5-C4-N3  | -4.80 | 120.67      | 128.46   |
| 2   | J     | 501 | DGT  | C5-C4-N3  | -4.80 | 120.68      | 128.46   |
| 2   | M     | 501 | DGT  | C5-C4-N3  | -4.76 | 120.74      | 128.46   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | A     | 501 | DGT  | C5-C4-N3 | -4.76 | 120.74      | 128.46   |
| 2   | E     | 501 | DGT  | C5-C4-N3 | -4.76 | 120.75      | 128.46   |
| 2   | N     | 501 | DGT  | C5-C4-N3 | -4.74 | 120.77      | 128.46   |
| 2   | F     | 501 | DGT  | C5-C4-N3 | -4.74 | 120.78      | 128.46   |
| 2   | K     | 501 | DGT  | C5-C4-N3 | -4.73 | 120.78      | 128.46   |
| 2   | C     | 501 | DGT  | C5-C4-N3 | -4.72 | 120.81      | 128.46   |
| 2   | L     | 501 | DGT  | C5-C4-N3 | -4.71 | 120.82      | 128.46   |
| 2   | I     | 501 | DGT  | C5-C4-N3 | -4.71 | 120.83      | 128.46   |
| 2   | D     | 501 | DGT  | C5-C4-N3 | -4.66 | 120.90      | 128.46   |
| 3   | K     | 502 | D5M  | N9-C8-N7 | -4.62 | 107.59      | 113.91   |
| 2   | P     | 501 | DGT  | C5-C4-N3 | -4.59 | 121.01      | 128.46   |
| 3   | L     | 502 | D5M  | N9-C8-N7 | -4.59 | 107.64      | 113.91   |
| 2   | G     | 501 | DGT  | C5-C4-N3 | -4.58 | 121.03      | 128.46   |
| 3   | O     | 502 | D5M  | N9-C8-N7 | -4.54 | 107.70      | 113.91   |
| 3   | A     | 502 | D5M  | N9-C8-N7 | -4.51 | 107.74      | 113.91   |
| 3   | J     | 502 | D5M  | N9-C8-N7 | -4.51 | 107.75      | 113.91   |
| 3   | I     | 502 | D5M  | N9-C8-N7 | -4.50 | 107.75      | 113.91   |
| 3   | G     | 502 | D5M  | N9-C8-N7 | -4.50 | 107.76      | 113.91   |
| 3   | N     | 502 | D5M  | N9-C8-N7 | -4.49 | 107.77      | 113.91   |
| 3   | P     | 502 | D5M  | N9-C8-N7 | -4.49 | 107.77      | 113.91   |
| 3   | B     | 502 | D5M  | N9-C8-N7 | -4.49 | 107.78      | 113.91   |
| 3   | E     | 502 | D5M  | N9-C8-N7 | -4.49 | 107.78      | 113.91   |
| 3   | D     | 502 | D5M  | N9-C8-N7 | -4.48 | 107.78      | 113.91   |
| 3   | H     | 502 | D5M  | N9-C8-N7 | -4.48 | 107.79      | 113.91   |
| 3   | M     | 502 | D5M  | N9-C8-N7 | -4.48 | 107.79      | 113.91   |
| 3   | C     | 502 | D5M  | N9-C8-N7 | -4.46 | 107.81      | 113.91   |
| 3   | F     | 502 | D5M  | N9-C8-N7 | -4.46 | 107.82      | 113.91   |
| 2   | B     | 501 | DGT  | C5-C4-N3 | -4.42 | 121.29      | 128.46   |
| 2   | O     | 501 | DGT  | C5-C4-N3 | -4.40 | 121.33      | 128.46   |
| 2   | K     | 501 | DGT  | C2-N3-C4 | 4.13  | 119.66      | 112.30   |
| 2   | M     | 501 | DGT  | C2-N3-C4 | 4.12  | 119.64      | 112.30   |
| 2   | I     | 501 | DGT  | C2-N3-C4 | 4.11  | 119.63      | 112.30   |
| 2   | A     | 501 | DGT  | C2-N3-C4 | 4.11  | 119.62      | 112.30   |
| 2   | E     | 501 | DGT  | C2-N3-C4 | 4.11  | 119.62      | 112.30   |
| 2   | H     | 501 | DGT  | C2-N3-C4 | 4.10  | 119.61      | 112.30   |
| 2   | J     | 501 | DGT  | C2-N3-C4 | 4.10  | 119.60      | 112.30   |
| 2   | L     | 501 | DGT  | C2-N3-C4 | 4.09  | 119.59      | 112.30   |
| 2   | F     | 501 | DGT  | C2-N3-C4 | 4.09  | 119.59      | 112.30   |
| 2   | N     | 501 | DGT  | C2-N3-C4 | 4.08  | 119.58      | 112.30   |
| 2   | C     | 501 | DGT  | C2-N3-C4 | 4.07  | 119.55      | 112.30   |
| 2   | G     | 501 | DGT  | C2-N3-C4 | 4.07  | 119.55      | 112.30   |
| 2   | D     | 501 | DGT  | C2-N3-C4 | 4.05  | 119.52      | 112.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | P     | 501 | DGT  | C2-N3-C4  | 4.05  | 119.51      | 112.30   |
| 2   | P     | 501 | DGT  | N9-C8-N7  | -3.97 | 105.91      | 113.39   |
| 2   | L     | 501 | DGT  | N9-C8-N7  | -3.94 | 105.96      | 113.39   |
| 2   | I     | 501 | DGT  | N9-C8-N7  | -3.94 | 105.97      | 113.39   |
| 2   | G     | 501 | DGT  | N9-C8-N7  | -3.92 | 106.00      | 113.39   |
| 2   | K     | 501 | DGT  | N9-C8-N7  | -3.89 | 106.06      | 113.39   |
| 2   | N     | 501 | DGT  | N9-C8-N7  | -3.87 | 106.10      | 113.39   |
| 2   | M     | 501 | DGT  | N9-C8-N7  | -3.87 | 106.10      | 113.39   |
| 2   | E     | 501 | DGT  | N9-C8-N7  | -3.87 | 106.11      | 113.39   |
| 2   | F     | 501 | DGT  | N9-C8-N7  | -3.85 | 106.13      | 113.39   |
| 2   | B     | 501 | DGT  | N9-C8-N7  | -3.85 | 106.13      | 113.39   |
| 2   | O     | 501 | DGT  | N9-C8-N7  | -3.85 | 106.14      | 113.39   |
| 2   | D     | 501 | DGT  | N9-C8-N7  | -3.85 | 106.15      | 113.39   |
| 2   | A     | 501 | DGT  | N9-C8-N7  | -3.84 | 106.16      | 113.39   |
| 2   | C     | 501 | DGT  | N9-C8-N7  | -3.84 | 106.16      | 113.39   |
| 2   | J     | 501 | DGT  | N9-C8-N7  | -3.83 | 106.18      | 113.39   |
| 2   | O     | 501 | DGT  | C2-N3-C4  | 3.83  | 119.12      | 112.30   |
| 2   | B     | 501 | DGT  | C2-N3-C4  | 3.82  | 119.11      | 112.30   |
| 2   | H     | 501 | DGT  | N9-C8-N7  | -3.79 | 106.26      | 113.39   |
| 2   | H     | 501 | DGT  | N9-C4-N3  | 3.56  | 133.09      | 125.94   |
| 2   | J     | 501 | DGT  | N9-C4-N3  | 3.56  | 133.08      | 125.94   |
| 3   | M     | 502 | D5M  | C2-N3-C4  | 3.53  | 120.10      | 111.75   |
| 2   | B     | 501 | DGT  | PA-O3A-PB | -3.53 | 120.71      | 132.83   |
| 2   | O     | 501 | DGT  | PA-O3A-PB | -3.53 | 120.72      | 132.83   |
| 3   | D     | 502 | D5M  | C2-N3-C4  | 3.52  | 120.08      | 111.75   |
| 3   | K     | 502 | D5M  | C5-N7-C8  | 3.52  | 108.51      | 103.51   |
| 3   | F     | 502 | D5M  | C2-N3-C4  | 3.52  | 120.06      | 111.75   |
| 3   | P     | 502 | D5M  | C2-N3-C4  | 3.52  | 120.06      | 111.75   |
| 3   | K     | 502 | D5M  | C2-N3-C4  | 3.51  | 120.05      | 111.75   |
| 3   | J     | 502 | D5M  | C2-N3-C4  | 3.51  | 120.05      | 111.75   |
| 2   | M     | 501 | DGT  | N9-C4-N3  | 3.51  | 132.99      | 125.94   |
| 2   | A     | 501 | DGT  | N9-C4-N3  | 3.51  | 132.98      | 125.94   |
| 2   | E     | 501 | DGT  | N9-C4-N3  | 3.50  | 132.97      | 125.94   |
| 3   | H     | 502 | D5M  | C2-N3-C4  | 3.50  | 120.02      | 111.75   |
| 3   | C     | 502 | D5M  | C2-N3-C4  | 3.50  | 120.02      | 111.75   |
| 2   | F     | 501 | DGT  | N9-C4-N3  | 3.50  | 132.96      | 125.94   |
| 3   | N     | 502 | D5M  | C2-N3-C4  | 3.50  | 120.01      | 111.75   |
| 3   | L     | 502 | D5M  | C2-N3-C4  | 3.50  | 120.01      | 111.75   |
| 3   | E     | 502 | D5M  | C2-N3-C4  | 3.49  | 120.00      | 111.75   |
| 2   | N     | 501 | DGT  | N9-C4-N3  | 3.49  | 132.95      | 125.94   |
| 3   | A     | 502 | D5M  | C2-N3-C4  | 3.49  | 119.99      | 111.75   |
| 3   | G     | 502 | D5M  | C2-N3-C4  | 3.49  | 119.99      | 111.75   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | C     | 501 | DGT  | N9-C4-N3  | 3.48  | 132.93      | 125.94   |
| 2   | K     | 501 | DGT  | N9-C4-N3  | 3.47  | 132.91      | 125.94   |
| 3   | B     | 502 | D5M  | C2-N3-C4  | 3.46  | 119.94      | 111.75   |
| 3   | O     | 502 | D5M  | C2-N3-C4  | 3.46  | 119.93      | 111.75   |
| 3   | I     | 502 | D5M  | C2-N3-C4  | 3.46  | 119.92      | 111.75   |
| 2   | L     | 501 | DGT  | N9-C4-N3  | 3.44  | 132.85      | 125.94   |
| 2   | I     | 501 | DGT  | N9-C4-N3  | 3.44  | 132.85      | 125.94   |
| 2   | D     | 501 | DGT  | N9-C4-N3  | 3.37  | 132.71      | 125.94   |
| 2   | P     | 501 | DGT  | N9-C4-N3  | 3.36  | 132.69      | 125.94   |
| 2   | I     | 501 | DGT  | PA-O3A-PB | -3.33 | 121.40      | 132.83   |
| 2   | G     | 501 | DGT  | N9-C4-N3  | 3.32  | 132.61      | 125.94   |
| 3   | L     | 502 | D5M  | C5-N7-C8  | 3.30  | 108.19      | 103.51   |
| 3   | K     | 502 | D5M  | N3-C4-N9  | 3.28  | 132.50      | 127.08   |
| 3   | O     | 502 | D5M  | C5-N7-C8  | 3.25  | 108.12      | 103.51   |
| 3   | F     | 502 | D5M  | C5-N7-C8  | 3.24  | 108.11      | 103.51   |
| 3   | D     | 502 | D5M  | C5-N7-C8  | 3.24  | 108.11      | 103.51   |
| 3   | C     | 502 | D5M  | C5-N7-C8  | 3.23  | 108.10      | 103.51   |
| 3   | J     | 502 | D5M  | C5-N7-C8  | 3.23  | 108.10      | 103.51   |
| 3   | A     | 502 | D5M  | C5-N7-C8  | 3.23  | 108.09      | 103.51   |
| 3   | P     | 502 | D5M  | C5-N7-C8  | 3.22  | 108.09      | 103.51   |
| 3   | G     | 502 | D5M  | C5-N7-C8  | 3.22  | 108.08      | 103.51   |
| 3   | E     | 502 | D5M  | C5-N7-C8  | 3.22  | 108.08      | 103.51   |
| 3   | E     | 502 | D5M  | N3-C4-N9  | 3.22  | 132.38      | 127.08   |
| 3   | I     | 502 | D5M  | C5-N7-C8  | 3.21  | 108.07      | 103.51   |
| 3   | H     | 502 | D5M  | C5-N7-C8  | 3.21  | 108.07      | 103.51   |
| 3   | B     | 502 | D5M  | C5-N7-C8  | 3.21  | 108.06      | 103.51   |
| 3   | N     | 502 | D5M  | C5-N7-C8  | 3.20  | 108.06      | 103.51   |
| 3   | M     | 502 | D5M  | C5-N7-C8  | 3.19  | 108.04      | 103.51   |
| 3   | N     | 502 | D5M  | N3-C4-N9  | 3.19  | 132.34      | 127.08   |
| 3   | C     | 502 | D5M  | N3-C4-N9  | 3.18  | 132.32      | 127.08   |
| 3   | F     | 502 | D5M  | N3-C4-N9  | 3.17  | 132.31      | 127.08   |
| 3   | H     | 502 | D5M  | N3-C4-N9  | 3.17  | 132.31      | 127.08   |
| 3   | J     | 502 | D5M  | N3-C4-N9  | 3.17  | 132.31      | 127.08   |
| 3   | L     | 502 | D5M  | N3-C4-N9  | 3.16  | 132.29      | 127.08   |
| 3   | M     | 502 | D5M  | N3-C4-N9  | 3.15  | 132.27      | 127.08   |
| 3   | A     | 502 | D5M  | N3-C4-N9  | 3.14  | 132.26      | 127.08   |
| 3   | G     | 502 | D5M  | N3-C4-N9  | 3.14  | 132.26      | 127.08   |
| 3   | B     | 502 | D5M  | N3-C4-N9  | 3.13  | 132.24      | 127.08   |
| 3   | O     | 502 | D5M  | N3-C4-N9  | 3.13  | 132.24      | 127.08   |
| 3   | P     | 502 | D5M  | N3-C4-N9  | 3.12  | 132.23      | 127.08   |
| 2   | L     | 501 | DGT  | PA-O3A-PB | -3.10 | 122.17      | 132.83   |
| 3   | I     | 502 | D5M  | N3-C4-N9  | 3.10  | 132.19      | 127.08   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | D     | 502 | D5M  | N3-C4-N9    | 3.07  | 132.15      | 127.08   |
| 2   | J     | 501 | DGT  | PA-O3A-PB   | -3.00 | 122.54      | 132.83   |
| 2   | H     | 501 | DGT  | PA-O3A-PB   | -3.00 | 122.55      | 132.83   |
| 2   | B     | 501 | DGT  | N9-C4-N3    | 2.97  | 131.90      | 125.94   |
| 2   | P     | 501 | DGT  | PA-O3A-PB   | -2.96 | 122.68      | 132.83   |
| 2   | O     | 501 | DGT  | N9-C4-N3    | 2.95  | 131.87      | 125.94   |
| 2   | D     | 501 | DGT  | PA-O3A-PB   | -2.95 | 122.70      | 132.83   |
| 2   | O     | 501 | DGT  | C2-N1-C6    | -2.94 | 119.74      | 125.10   |
| 2   | B     | 501 | DGT  | C2-N1-C6    | -2.93 | 119.75      | 125.10   |
| 2   | E     | 501 | DGT  | PA-O3A-PB   | -2.93 | 122.77      | 132.83   |
| 2   | M     | 501 | DGT  | PA-O3A-PB   | -2.93 | 122.77      | 132.83   |
| 2   | I     | 501 | DGT  | C2-N1-C6    | -2.93 | 119.76      | 125.10   |
| 2   | N     | 501 | DGT  | PA-O3A-PB   | -2.93 | 122.77      | 132.83   |
| 2   | C     | 501 | DGT  | C2-N1-C6    | -2.93 | 119.76      | 125.10   |
| 2   | A     | 501 | DGT  | PA-O3A-PB   | -2.93 | 122.78      | 132.83   |
| 2   | F     | 501 | DGT  | PA-O3A-PB   | -2.92 | 122.79      | 132.83   |
| 2   | G     | 501 | DGT  | PA-O3A-PB   | -2.92 | 122.80      | 132.83   |
| 2   | F     | 501 | DGT  | C2-N1-C6    | -2.91 | 119.78      | 125.10   |
| 2   | N     | 501 | DGT  | C2-N1-C6    | -2.90 | 119.81      | 125.10   |
| 2   | K     | 501 | DGT  | C2-N1-C6    | -2.90 | 119.81      | 125.10   |
| 2   | M     | 501 | DGT  | C2-N1-C6    | -2.90 | 119.82      | 125.10   |
| 2   | A     | 501 | DGT  | C2-N1-C6    | -2.89 | 119.83      | 125.10   |
| 2   | L     | 501 | DGT  | C2-N1-C6    | -2.89 | 119.84      | 125.10   |
| 2   | E     | 501 | DGT  | C2-N1-C6    | -2.88 | 119.84      | 125.10   |
| 2   | D     | 501 | DGT  | C2-N1-C6    | -2.87 | 119.86      | 125.10   |
| 2   | J     | 501 | DGT  | C2-N1-C6    | -2.86 | 119.88      | 125.10   |
| 2   | H     | 501 | DGT  | C2-N1-C6    | -2.86 | 119.88      | 125.10   |
| 2   | G     | 501 | DGT  | C2-N1-C6    | -2.86 | 119.89      | 125.10   |
| 2   | P     | 501 | DGT  | C2-N1-C6    | -2.84 | 119.92      | 125.10   |
| 2   | B     | 501 | DGT  | PB-O3B-PG   | -2.82 | 123.16      | 132.83   |
| 2   | O     | 501 | DGT  | PB-O3B-PG   | -2.81 | 123.18      | 132.83   |
| 2   | C     | 501 | DGT  | PA-O3A-PB   | -2.80 | 123.20      | 132.83   |
| 2   | P     | 501 | DGT  | C4'-O4'-C1' | -2.80 | 102.67      | 109.45   |
| 2   | G     | 501 | DGT  | PB-O3B-PG   | -2.75 | 123.40      | 132.83   |
| 2   | K     | 501 | DGT  | PA-O3A-PB   | -2.74 | 123.41      | 132.83   |
| 2   | I     | 501 | DGT  | C5-C6-N1    | 2.74  | 120.14      | 113.19   |
| 2   | L     | 501 | DGT  | C5-C6-N1    | 2.73  | 120.12      | 113.19   |
| 2   | J     | 501 | DGT  | C5-C6-N1    | 2.72  | 120.10      | 113.19   |
| 2   | K     | 501 | DGT  | C5-C6-N1    | 2.72  | 120.09      | 113.19   |
| 2   | F     | 501 | DGT  | C5-C6-N1    | 2.72  | 120.09      | 113.19   |
| 3   | F     | 502 | D5M  | C2'-C3'-C4' | 2.71  | 108.42      | 102.76   |
| 2   | H     | 501 | DGT  | C5-C6-N1    | 2.71  | 120.08      | 113.19   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 501 | DGT  | C5-C6-N1    | 2.71  | 120.07      | 113.19   |
| 2   | H     | 501 | DGT  | PB-O3B-PG   | -2.71 | 123.53      | 132.83   |
| 2   | N     | 501 | DGT  | C5-C6-N1    | 2.71  | 120.06      | 113.19   |
| 2   | J     | 501 | DGT  | PB-O3B-PG   | -2.71 | 123.54      | 132.83   |
| 2   | G     | 501 | DGT  | C5-C6-N1    | 2.71  | 120.06      | 113.19   |
| 2   | C     | 501 | DGT  | C5-C6-N1    | 2.70  | 120.05      | 113.19   |
| 2   | E     | 501 | DGT  | C5-C6-N1    | 2.70  | 120.05      | 113.19   |
| 2   | M     | 501 | DGT  | C5-C6-N1    | 2.70  | 120.05      | 113.19   |
| 2   | D     | 501 | DGT  | PB-O3B-PG   | -2.69 | 123.60      | 132.83   |
| 2   | P     | 501 | DGT  | C5-C6-N1    | 2.67  | 119.97      | 113.19   |
| 2   | D     | 501 | DGT  | C5-C6-N1    | 2.67  | 119.96      | 113.19   |
| 2   | G     | 501 | DGT  | C4'-O4'-C1' | -2.66 | 103.02      | 109.45   |
| 2   | C     | 501 | DGT  | PB-O3B-PG   | -2.64 | 123.77      | 132.83   |
| 2   | P     | 501 | DGT  | PB-O3B-PG   | -2.63 | 123.82      | 132.83   |
| 2   | F     | 501 | DGT  | PB-O3B-PG   | -2.61 | 123.87      | 132.83   |
| 2   | E     | 501 | DGT  | PB-O3B-PG   | -2.61 | 123.88      | 132.83   |
| 2   | K     | 501 | DGT  | PB-O3B-PG   | -2.60 | 123.89      | 132.83   |
| 2   | M     | 501 | DGT  | PB-O3B-PG   | -2.60 | 123.90      | 132.83   |
| 2   | N     | 501 | DGT  | PB-O3B-PG   | -2.60 | 123.90      | 132.83   |
| 2   | A     | 501 | DGT  | PB-O3B-PG   | -2.60 | 123.91      | 132.83   |
| 3   | D     | 502 | D5M  | C2'-C3'-C4' | 2.59  | 108.16      | 102.76   |
| 2   | O     | 501 | DGT  | C5-C6-N1    | 2.58  | 119.75      | 113.19   |
| 2   | B     | 501 | DGT  | C5-C6-N1    | 2.58  | 119.74      | 113.19   |
| 2   | I     | 501 | DGT  | PB-O3B-PG   | -2.57 | 124.02      | 132.83   |
| 2   | P     | 501 | DGT  | C8-N7-C5    | 2.55  | 108.86      | 104.24   |
| 2   | N     | 501 | DGT  | C8-N7-C5    | 2.55  | 108.85      | 104.24   |
| 2   | E     | 501 | DGT  | C8-N7-C5    | 2.55  | 108.85      | 104.24   |
| 2   | I     | 501 | DGT  | C8-N7-C5    | 2.54  | 108.84      | 104.24   |
| 2   | F     | 501 | DGT  | C8-N7-C5    | 2.54  | 108.84      | 104.24   |
| 2   | L     | 501 | DGT  | C8-N7-C5    | 2.54  | 108.83      | 104.24   |
| 2   | M     | 501 | DGT  | C8-N7-C5    | 2.54  | 108.83      | 104.24   |
| 2   | K     | 501 | DGT  | C8-N7-C5    | 2.53  | 108.82      | 104.24   |
| 2   | A     | 501 | DGT  | C8-N7-C5    | 2.53  | 108.82      | 104.24   |
| 2   | E     | 501 | DGT  | O6-C6-C5    | -2.52 | 119.91      | 126.60   |
| 2   | G     | 501 | DGT  | C8-N7-C5    | 2.52  | 108.81      | 104.24   |
| 2   | A     | 501 | DGT  | O6-C6-C5    | -2.52 | 119.91      | 126.60   |
| 3   | B     | 502 | D5M  | C2'-C3'-C4' | 2.52  | 108.01      | 102.76   |
| 2   | G     | 501 | DGT  | O6-C6-C5    | -2.52 | 119.92      | 126.60   |
| 2   | N     | 501 | DGT  | O6-C6-C5    | -2.51 | 119.93      | 126.60   |
| 2   | M     | 501 | DGT  | O6-C6-C5    | -2.51 | 119.93      | 126.60   |
| 2   | I     | 501 | DGT  | O6-C6-C5    | -2.51 | 119.94      | 126.60   |
| 2   | J     | 501 | DGT  | C8-N7-C5    | 2.51  | 108.78      | 104.24   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | F     | 501 | DGT  | O6-C6-C5    | -2.51 | 119.94      | 126.60   |
| 2   | K     | 501 | DGT  | O6-C6-C5    | -2.49 | 120.01      | 126.60   |
| 2   | D     | 501 | DGT  | C8-N7-C5    | 2.49  | 108.74      | 104.24   |
| 2   | H     | 501 | DGT  | C8-N7-C5    | 2.49  | 108.74      | 104.24   |
| 2   | J     | 501 | DGT  | O6-C6-C5    | -2.48 | 120.01      | 126.60   |
| 2   | L     | 501 | DGT  | O6-C6-C5    | -2.48 | 120.02      | 126.60   |
| 2   | C     | 501 | DGT  | C8-N7-C5    | 2.48  | 108.73      | 104.24   |
| 2   | C     | 501 | DGT  | O6-C6-C5    | -2.48 | 120.03      | 126.60   |
| 2   | O     | 501 | DGT  | C8-N7-C5    | 2.47  | 108.72      | 104.24   |
| 2   | B     | 501 | DGT  | C8-N7-C5    | 2.47  | 108.71      | 104.24   |
| 3   | H     | 502 | D5M  | C3'-C2'-C1' | 2.46  | 108.71      | 102.54   |
| 2   | D     | 501 | DGT  | O6-C6-C5    | -2.46 | 120.07      | 126.60   |
| 2   | H     | 501 | DGT  | O6-C6-C5    | -2.46 | 120.07      | 126.60   |
| 3   | I     | 502 | D5M  | C2'-C3'-C4' | 2.46  | 107.88      | 102.76   |
| 2   | P     | 501 | DGT  | O6-C6-C5    | -2.44 | 120.12      | 126.60   |
| 2   | L     | 501 | DGT  | PB-O3B-PG   | -2.44 | 124.45      | 132.83   |
| 3   | O     | 502 | D5M  | C4-N9-C8    | 2.43  | 108.36      | 105.73   |
| 2   | P     | 501 | DGT  | C8-N9-C4    | 2.43  | 110.67      | 106.05   |
| 3   | J     | 502 | D5M  | C4-N9-C8    | 2.41  | 108.34      | 105.73   |
| 3   | K     | 502 | D5M  | C4-N9-C8    | 2.41  | 108.34      | 105.73   |
| 3   | E     | 502 | D5M  | C3'-C2'-C1' | 2.41  | 108.57      | 102.54   |
| 3   | A     | 502 | D5M  | C4-N9-C8    | 2.41  | 108.33      | 105.73   |
| 3   | M     | 502 | D5M  | C4-N9-C8    | 2.41  | 108.33      | 105.73   |
| 2   | G     | 501 | DGT  | C8-N9-C4    | 2.40  | 110.62      | 106.05   |
| 3   | C     | 502 | D5M  | C3'-C2'-C1' | 2.40  | 108.55      | 102.54   |
| 3   | L     | 502 | D5M  | C4-N9-C8    | 2.40  | 108.33      | 105.73   |
| 3   | N     | 502 | D5M  | C4-N9-C8    | 2.40  | 108.33      | 105.73   |
| 3   | I     | 502 | D5M  | C4-N9-C8    | 2.39  | 108.32      | 105.73   |
| 3   | G     | 502 | D5M  | C4-N9-C8    | 2.39  | 108.31      | 105.73   |
| 2   | I     | 501 | DGT  | C8-N9-C4    | 2.38  | 110.58      | 106.05   |
| 3   | E     | 502 | D5M  | C4-N9-C8    | 2.38  | 108.31      | 105.73   |
| 3   | P     | 502 | D5M  | C4-N9-C8    | 2.38  | 108.30      | 105.73   |
| 3   | K     | 502 | D5M  | C4-C5-N7    | -2.37 | 107.73      | 110.62   |
| 2   | B     | 501 | DGT  | O6-C6-C5    | -2.37 | 120.33      | 126.60   |
| 2   | L     | 501 | DGT  | C8-N9-C4    | 2.36  | 110.55      | 106.05   |
| 2   | O     | 501 | DGT  | O6-C6-C5    | -2.36 | 120.34      | 126.60   |
| 3   | B     | 502 | D5M  | C4-N9-C8    | 2.36  | 108.28      | 105.73   |
| 3   | C     | 502 | D5M  | C4-N9-C8    | 2.35  | 108.27      | 105.73   |
| 2   | M     | 501 | DGT  | C8-N9-C4    | 2.34  | 110.50      | 106.05   |
| 3   | H     | 502 | D5M  | C2'-C3'-C4' | 2.33  | 107.63      | 102.76   |
| 2   | N     | 501 | DGT  | C8-N9-C4    | 2.33  | 110.49      | 106.05   |
| 3   | H     | 502 | D5M  | C4-N9-C8    | 2.33  | 108.25      | 105.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | E     | 501 | DGT  | C8-N9-C4    | 2.33  | 110.48      | 106.05   |
| 2   | K     | 501 | DGT  | C8-N9-C4    | 2.33  | 110.48      | 106.05   |
| 2   | C     | 501 | DGT  | C8-N9-C4    | 2.32  | 110.47      | 106.05   |
| 2   | F     | 501 | DGT  | C8-N9-C4    | 2.32  | 110.46      | 106.05   |
| 3   | O     | 502 | D5M  | C3'-C2'-C1' | 2.32  | 108.34      | 102.54   |
| 2   | A     | 501 | DGT  | C8-N9-C4    | 2.32  | 110.46      | 106.05   |
| 2   | J     | 501 | DGT  | C8-N9-C4    | 2.31  | 110.45      | 106.05   |
| 2   | D     | 501 | DGT  | C8-N9-C4    | 2.31  | 110.45      | 106.05   |
| 3   | O     | 502 | D5M  | C2'-C3'-C4' | 2.31  | 107.57      | 102.76   |
| 3   | F     | 502 | D5M  | C4-N9-C8    | 2.30  | 108.22      | 105.73   |
| 2   | H     | 501 | DGT  | C8-N9-C4    | 2.30  | 110.43      | 106.05   |
| 3   | D     | 502 | D5M  | C4-N9-C8    | 2.29  | 108.21      | 105.73   |
| 3   | I     | 502 | D5M  | C3'-C2'-C1' | 2.28  | 108.24      | 102.54   |
| 3   | C     | 502 | D5M  | C2'-C3'-C4' | 2.25  | 107.46      | 102.76   |
| 3   | J     | 502 | D5M  | C3'-C2'-C1' | 2.25  | 108.17      | 102.54   |
| 3   | M     | 502 | D5M  | C3'-C2'-C1' | 2.24  | 108.15      | 102.54   |
| 2   | B     | 501 | DGT  | C8-N9-C4    | 2.22  | 110.28      | 106.05   |
| 2   | O     | 501 | DGT  | C8-N9-C4    | 2.21  | 110.25      | 106.05   |
| 3   | K     | 502 | D5M  | C6-C5-C4    | 2.19  | 120.12      | 117.18   |
| 3   | K     | 502 | D5M  | C4'-O4'-C1' | -2.18 | 104.19      | 109.45   |
| 3   | F     | 502 | D5M  | C3'-C2'-C1' | 2.16  | 107.96      | 102.54   |
| 3   | D     | 502 | D5M  | C4-C5-N7    | -2.15 | 108.00      | 110.62   |
| 3   | G     | 502 | D5M  | C3'-C2'-C1' | 2.14  | 107.89      | 102.54   |
| 3   | O     | 502 | D5M  | C4-C5-N7    | -2.13 | 108.02      | 110.62   |
| 3   | A     | 502 | D5M  | C3'-C2'-C1' | 2.13  | 107.87      | 102.54   |
| 3   | N     | 502 | D5M  | C2'-C1'-N9  | -2.12 | 109.30      | 114.28   |
| 3   | P     | 502 | D5M  | C2'-C1'-N9  | -2.11 | 109.32      | 114.28   |
| 3   | F     | 502 | D5M  | C4-C5-N7    | -2.11 | 108.05      | 110.62   |
| 3   | L     | 502 | D5M  | C4-C5-N7    | -2.11 | 108.05      | 110.62   |
| 3   | J     | 502 | D5M  | C2'-C1'-N9  | -2.10 | 109.35      | 114.28   |
| 3   | P     | 502 | D5M  | C4-C5-N7    | -2.09 | 108.07      | 110.62   |
| 3   | A     | 502 | D5M  | C4-C5-N7    | -2.08 | 108.08      | 110.62   |
| 3   | I     | 502 | D5M  | C4-C5-N7    | -2.08 | 108.08      | 110.62   |
| 3   | C     | 502 | D5M  | C4-C5-N7    | -2.08 | 108.08      | 110.62   |
| 3   | J     | 502 | D5M  | C4-C5-N7    | -2.08 | 108.09      | 110.62   |
| 3   | G     | 502 | D5M  | C4-C5-N7    | -2.07 | 108.09      | 110.62   |
| 3   | E     | 502 | D5M  | C2'-C3'-C4' | 2.07  | 107.07      | 102.76   |
| 3   | N     | 502 | D5M  | C3'-C2'-C1' | 2.06  | 107.70      | 102.54   |
| 3   | M     | 502 | D5M  | C4-C5-N7    | -2.06 | 108.11      | 110.62   |
| 3   | N     | 502 | D5M  | C4-C5-N7    | -2.05 | 108.13      | 110.62   |
| 3   | H     | 502 | D5M  | C4-C5-N7    | -2.05 | 108.13      | 110.62   |
| 3   | B     | 502 | D5M  | C2'-C1'-N9  | -2.04 | 109.49      | 114.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | D     | 502 | D5M  | C3'-C2'-C1' | 2.04  | 107.65      | 102.54   |
| 3   | B     | 502 | D5M  | C4-C5-N7    | -2.04 | 108.13      | 110.62   |
| 3   | E     | 502 | D5M  | C4-C5-N7    | -2.02 | 108.15      | 110.62   |
| 3   | E     | 502 | D5M  | C6-C5-C4    | 2.01  | 119.88      | 117.18   |
| 3   | N     | 502 | D5M  | C6-C5-C4    | 2.00  | 119.88      | 117.18   |
| 2   | C     | 501 | DGT  | C4'-O4'-C1' | -2.00 | 104.61      | 109.45   |

There are no chirality outliers.

All (164) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 501 | DGT  | C5'-O5'-PA-O1A  |
| 2   | A     | 501 | DGT  | C5'-O5'-PA-O2A  |
| 2   | A     | 501 | DGT  | O4'-C4'-C5'-O5' |
| 2   | B     | 501 | DGT  | C5'-O5'-PA-O1A  |
| 2   | B     | 501 | DGT  | C5'-O5'-PA-O2A  |
| 2   | B     | 501 | DGT  | O4'-C4'-C5'-O5' |
| 2   | C     | 501 | DGT  | C5'-O5'-PA-O1A  |
| 2   | C     | 501 | DGT  | C5'-O5'-PA-O2A  |
| 2   | C     | 501 | DGT  | O4'-C4'-C5'-O5' |
| 2   | D     | 501 | DGT  | O4'-C4'-C5'-O5' |
| 2   | D     | 501 | DGT  | C3'-C4'-C5'-O5' |
| 2   | E     | 501 | DGT  | C5'-O5'-PA-O1A  |
| 2   | E     | 501 | DGT  | C5'-O5'-PA-O2A  |
| 2   | E     | 501 | DGT  | O4'-C4'-C5'-O5' |
| 2   | F     | 501 | DGT  | C5'-O5'-PA-O1A  |
| 2   | F     | 501 | DGT  | C5'-O5'-PA-O2A  |
| 2   | F     | 501 | DGT  | O4'-C4'-C5'-O5' |
| 2   | G     | 501 | DGT  | C5'-O5'-PA-O3A  |
| 2   | G     | 501 | DGT  | C5'-O5'-PA-O2A  |
| 2   | G     | 501 | DGT  | C3'-C4'-C5'-O5' |
| 2   | H     | 501 | DGT  | C5'-O5'-PA-O3A  |
| 2   | H     | 501 | DGT  | C5'-O5'-PA-O1A  |
| 2   | I     | 501 | DGT  | O4'-C4'-C5'-O5' |
| 2   | J     | 501 | DGT  | C5'-O5'-PA-O3A  |
| 2   | J     | 501 | DGT  | C5'-O5'-PA-O1A  |
| 2   | K     | 501 | DGT  | C5'-O5'-PA-O1A  |
| 2   | K     | 501 | DGT  | C5'-O5'-PA-O2A  |
| 2   | K     | 501 | DGT  | O4'-C4'-C5'-O5' |
| 2   | K     | 501 | DGT  | C3'-C4'-C5'-O5' |
| 2   | L     | 501 | DGT  | PB-O3B-PG-O2G   |
| 2   | L     | 501 | DGT  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | L     | 501 | DGT  | C3'-C4'-C5'-O5' |
| 2   | M     | 501 | DGT  | C5'-O5'-PA-O1A  |
| 2   | M     | 501 | DGT  | C5'-O5'-PA-O2A  |
| 2   | M     | 501 | DGT  | O4'-C4'-C5'-O5' |
| 2   | N     | 501 | DGT  | C5'-O5'-PA-O1A  |
| 2   | N     | 501 | DGT  | C5'-O5'-PA-O2A  |
| 2   | N     | 501 | DGT  | O4'-C4'-C5'-O5' |
| 2   | O     | 501 | DGT  | C5'-O5'-PA-O1A  |
| 2   | O     | 501 | DGT  | C5'-O5'-PA-O2A  |
| 2   | O     | 501 | DGT  | O4'-C4'-C5'-O5' |
| 2   | P     | 501 | DGT  | C5'-O5'-PA-O2A  |
| 3   | A     | 502 | D5M  | C5'-O5'-P-O3P   |
| 3   | A     | 502 | D5M  | C5'-O5'-P-O2P   |
| 3   | B     | 502 | D5M  | C5'-O5'-P-O3P   |
| 3   | B     | 502 | D5M  | C5'-O5'-P-O2P   |
| 3   | C     | 502 | D5M  | C5'-O5'-P-O3P   |
| 3   | C     | 502 | D5M  | C5'-O5'-P-O2P   |
| 3   | D     | 502 | D5M  | C5'-O5'-P-O1P   |
| 3   | D     | 502 | D5M  | C5'-O5'-P-O3P   |
| 3   | D     | 502 | D5M  | C5'-O5'-P-O2P   |
| 3   | E     | 502 | D5M  | C5'-O5'-P-O2P   |
| 3   | F     | 502 | D5M  | C5'-O5'-P-O3P   |
| 3   | F     | 502 | D5M  | C5'-O5'-P-O2P   |
| 3   | G     | 502 | D5M  | C5'-O5'-P-O3P   |
| 3   | G     | 502 | D5M  | C5'-O5'-P-O2P   |
| 3   | H     | 502 | D5M  | C5'-O5'-P-O3P   |
| 3   | H     | 502 | D5M  | C5'-O5'-P-O2P   |
| 3   | I     | 502 | D5M  | O4'-C4'-C5'-O5' |
| 3   | J     | 502 | D5M  | O4'-C4'-C5'-O5' |
| 3   | K     | 502 | D5M  | O4'-C4'-C5'-O5' |
| 3   | K     | 502 | D5M  | C3'-C4'-C5'-O5' |
| 3   | L     | 502 | D5M  | O4'-C4'-C5'-O5' |
| 3   | M     | 502 | D5M  | C5'-O5'-P-O1P   |
| 3   | M     | 502 | D5M  | C5'-O5'-P-O2P   |
| 2   | A     | 501 | DGT  | C3'-C4'-C5'-O5' |
| 2   | B     | 501 | DGT  | C3'-C4'-C5'-O5' |
| 2   | C     | 501 | DGT  | C3'-C4'-C5'-O5' |
| 2   | E     | 501 | DGT  | C3'-C4'-C5'-O5' |
| 2   | F     | 501 | DGT  | C3'-C4'-C5'-O5' |
| 2   | G     | 501 | DGT  | O4'-C4'-C5'-O5' |
| 2   | H     | 501 | DGT  | C3'-C4'-C5'-O5' |
| 2   | M     | 501 | DGT  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | N     | 501 | DGT  | C3'-C4'-C5'-O5' |
| 2   | O     | 501 | DGT  | C3'-C4'-C5'-O5' |
| 3   | L     | 502 | D5M  | C3'-C4'-C5'-O5' |
| 3   | N     | 502 | D5M  | O4'-C4'-C5'-O5' |
| 3   | P     | 502 | D5M  | O4'-C4'-C5'-O5' |
| 2   | I     | 501 | DGT  | C3'-C4'-C5'-O5' |
| 2   | J     | 501 | DGT  | C3'-C4'-C5'-O5' |
| 3   | I     | 502 | D5M  | C3'-C4'-C5'-O5' |
| 3   | O     | 502 | D5M  | O4'-C4'-C5'-O5' |
| 3   | O     | 502 | D5M  | C3'-C4'-C5'-O5' |
| 3   | A     | 502 | D5M  | C5'-O5'-P-O1P   |
| 3   | B     | 502 | D5M  | C5'-O5'-P-O1P   |
| 3   | C     | 502 | D5M  | C5'-O5'-P-O1P   |
| 3   | E     | 502 | D5M  | C5'-O5'-P-O1P   |
| 3   | F     | 502 | D5M  | C5'-O5'-P-O1P   |
| 3   | G     | 502 | D5M  | C5'-O5'-P-O1P   |
| 3   | H     | 502 | D5M  | C5'-O5'-P-O1P   |
| 2   | B     | 501 | DGT  | PA-O3A-PB-O2B   |
| 2   | I     | 501 | DGT  | PA-O3A-PB-O2B   |
| 2   | K     | 501 | DGT  | PG-O3B-PB-O2B   |
| 2   | O     | 501 | DGT  | PA-O3A-PB-O2B   |
| 2   | H     | 501 | DGT  | O4'-C4'-C5'-O5' |
| 2   | J     | 501 | DGT  | O4'-C4'-C5'-O5' |
| 2   | A     | 501 | DGT  | PG-O3B-PB-O3A   |
| 2   | E     | 501 | DGT  | PG-O3B-PB-O3A   |
| 2   | F     | 501 | DGT  | PG-O3B-PB-O3A   |
| 2   | M     | 501 | DGT  | PG-O3B-PB-O3A   |
| 2   | N     | 501 | DGT  | PG-O3B-PB-O3A   |
| 2   | K     | 501 | DGT  | C4'-C5'-O5'-PA  |
| 2   | C     | 501 | DGT  | PB-O3A-PA-O5'   |
| 2   | K     | 501 | DGT  | PB-O3A-PA-O5'   |
| 3   | A     | 502 | D5M  | C2'-C1'-N9-C4   |
| 3   | E     | 502 | D5M  | C5'-O5'-P-O3P   |
| 3   | E     | 502 | D5M  | C2'-C1'-N9-C4   |
| 3   | H     | 502 | D5M  | C2'-C1'-N9-C4   |
| 3   | N     | 502 | D5M  | C2'-C1'-N9-C4   |
| 3   | P     | 502 | D5M  | C2'-C1'-N9-C4   |
| 2   | H     | 501 | DGT  | PB-O3B-PG-O3G   |
| 2   | J     | 501 | DGT  | PB-O3B-PG-O3G   |
| 2   | A     | 501 | DGT  | C5'-O5'-PA-O3A  |
| 2   | C     | 501 | DGT  | C5'-O5'-PA-O3A  |
| 2   | E     | 501 | DGT  | C5'-O5'-PA-O3A  |

*Continued on next page...*

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | F     | 501 | DGT  | C5'-O5'-PA-O3A  |
| 2   | M     | 501 | DGT  | C5'-O5'-PA-O3A  |
| 2   | N     | 501 | DGT  | C5'-O5'-PA-O3A  |
| 2   | P     | 501 | DGT  | C5'-O5'-PA-O3A  |
| 3   | N     | 502 | D5M  | C3'-C4'-C5'-O5' |
| 3   | P     | 502 | D5M  | C3'-C4'-C5'-O5' |
| 2   | P     | 501 | DGT  | PA-O3A-PB-O2B   |
| 2   | H     | 501 | DGT  | C5'-O5'-PA-O2A  |
| 2   | J     | 501 | DGT  | C5'-O5'-PA-O2A  |
| 2   | A     | 501 | DGT  | PB-O3A-PA-O2A   |
| 2   | D     | 501 | DGT  | PA-O3A-PB-O2B   |
| 2   | E     | 501 | DGT  | PB-O3A-PA-O2A   |
| 2   | F     | 501 | DGT  | PB-O3A-PA-O2A   |
| 2   | M     | 501 | DGT  | PB-O3A-PA-O2A   |
| 2   | N     | 501 | DGT  | PB-O3A-PA-O2A   |
| 3   | M     | 502 | D5M  | O4'-C4'-C5'-O5' |
| 2   | A     | 501 | DGT  | PB-O3A-PA-O5'   |
| 2   | E     | 501 | DGT  | PB-O3A-PA-O5'   |
| 2   | F     | 501 | DGT  | PB-O3A-PA-O5'   |
| 2   | M     | 501 | DGT  | PB-O3A-PA-O5'   |
| 2   | N     | 501 | DGT  | PB-O3A-PA-O5'   |
| 3   | C     | 502 | D5M  | C2'-C1'-N9-C4   |
| 3   | G     | 502 | D5M  | C2'-C1'-N9-C4   |
| 3   | J     | 502 | D5M  | C2'-C1'-N9-C4   |
| 3   | L     | 502 | D5M  | C5'-O5'-P-O3P   |
| 3   | M     | 502 | D5M  | C5'-O5'-P-O3P   |
| 3   | M     | 502 | D5M  | C2'-C1'-N9-C4   |
| 2   | D     | 501 | DGT  | PB-O3B-PG-O1G   |
| 2   | H     | 501 | DGT  | PB-O3B-PG-O1G   |
| 2   | H     | 501 | DGT  | PB-O3B-PG-O2G   |
| 2   | J     | 501 | DGT  | PB-O3B-PG-O1G   |
| 2   | J     | 501 | DGT  | PB-O3B-PG-O2G   |
| 2   | B     | 501 | DGT  | C5'-O5'-PA-O3A  |
| 2   | K     | 501 | DGT  | C5'-O5'-PA-O3A  |
| 2   | O     | 501 | DGT  | C5'-O5'-PA-O3A  |
| 3   | A     | 502 | D5M  | O4'-C4'-C5'-O5' |
| 3   | C     | 502 | D5M  | O4'-C4'-C5'-O5' |
| 3   | D     | 502 | D5M  | O4'-C4'-C5'-O5' |
| 3   | E     | 502 | D5M  | O4'-C4'-C5'-O5' |
| 3   | H     | 502 | D5M  | O4'-C4'-C5'-O5' |
| 2   | A     | 501 | DGT  | PG-O3B-PB-O2B   |
| 2   | E     | 501 | DGT  | PG-O3B-PB-O2B   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | F     | 501 | DGT  | PG-O3B-PB-O2B   |
| 2   | M     | 501 | DGT  | PG-O3B-PB-O2B   |
| 2   | N     | 501 | DGT  | PG-O3B-PB-O2B   |
| 3   | F     | 502 | D5M  | O4'-C4'-C5'-O5' |
| 3   | G     | 502 | D5M  | O4'-C4'-C5'-O5' |
| 2   | L     | 501 | DGT  | PB-O3B-PG-O3G   |
| 3   | J     | 502 | D5M  | C3'-C4'-C5'-O5' |

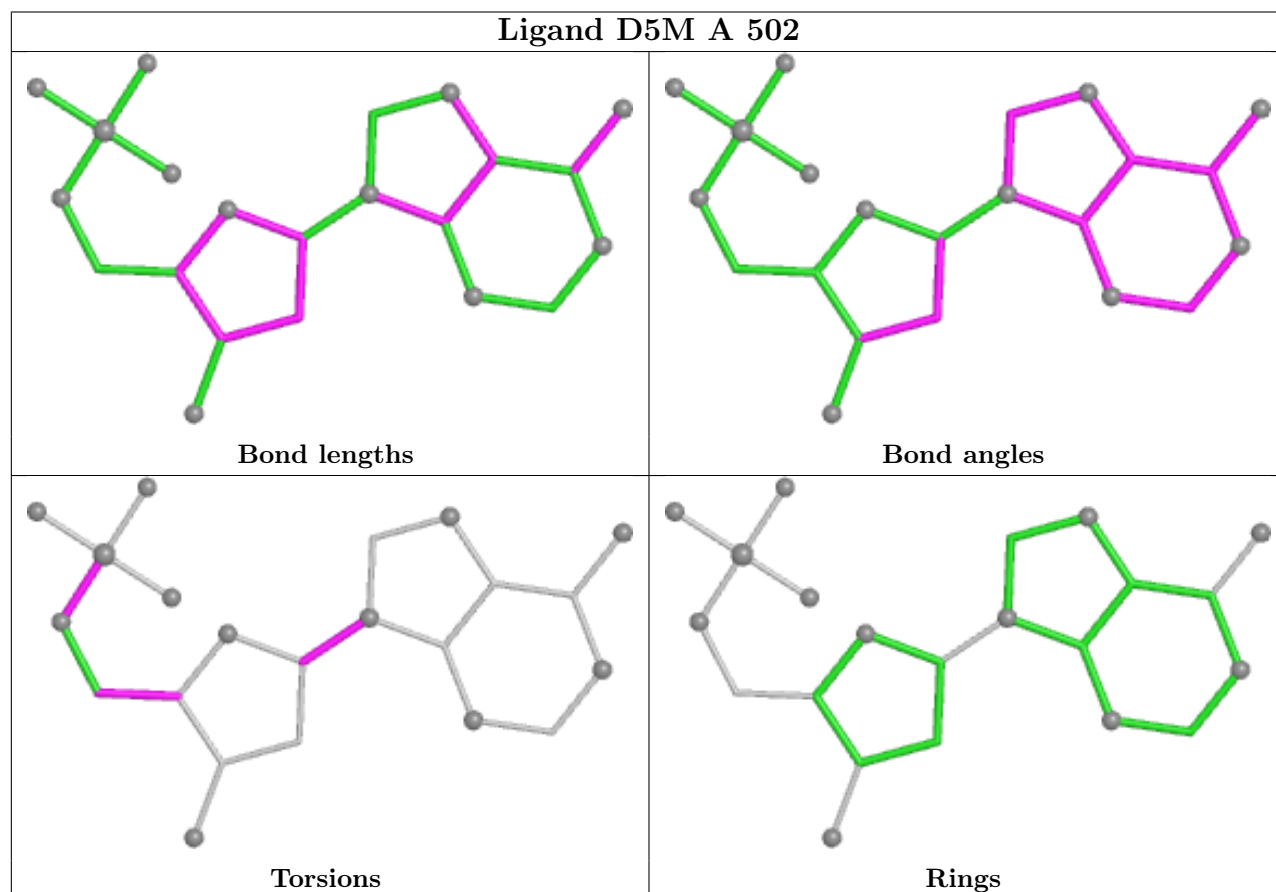
There are no ring outliers.

25 monomers are involved in 47 short contacts:

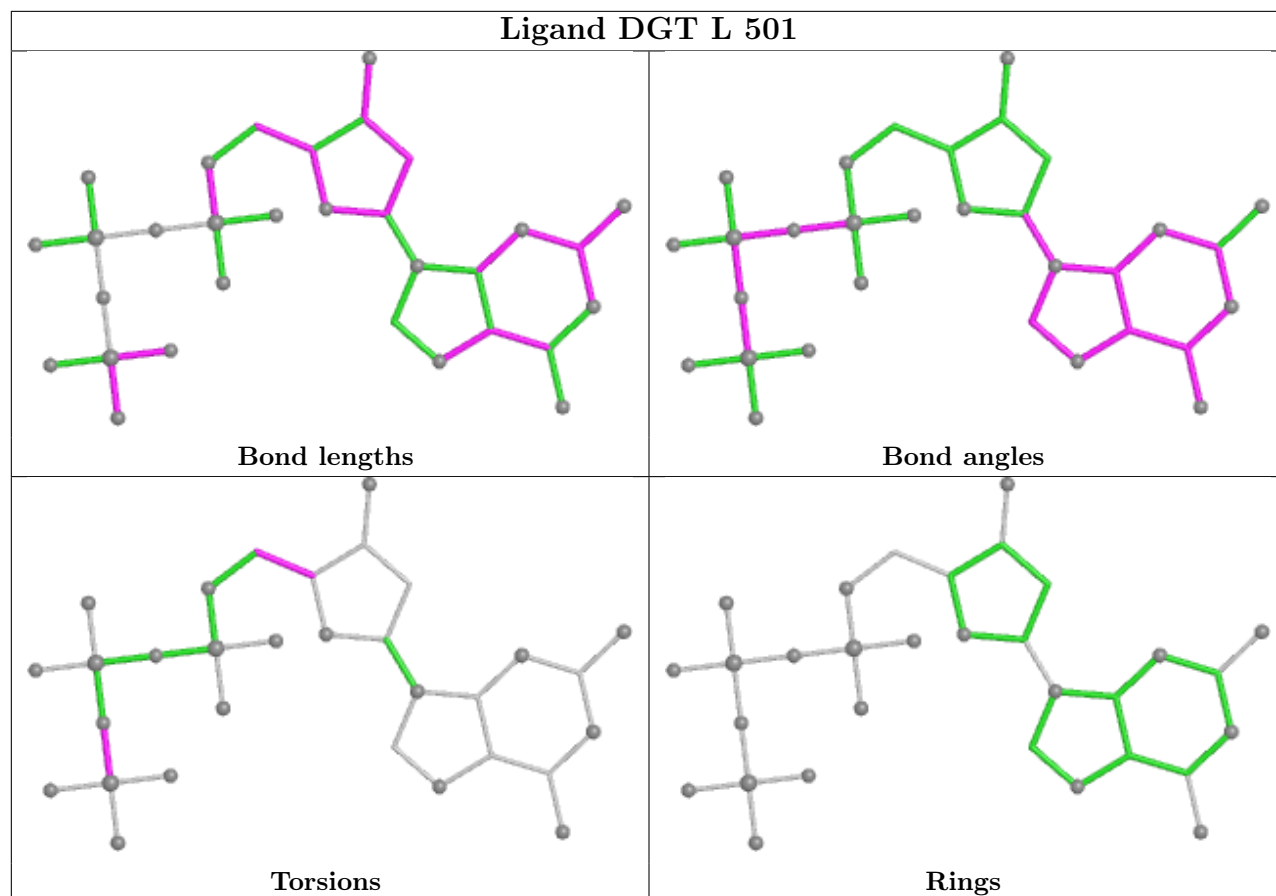
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 502 | D5M  | 1       | 0            |
| 2   | L     | 501 | DGT  | 2       | 0            |
| 2   | G     | 501 | DGT  | 3       | 0            |
| 2   | E     | 501 | DGT  | 2       | 0            |
| 2   | I     | 501 | DGT  | 2       | 0            |
| 2   | O     | 501 | DGT  | 6       | 0            |
| 3   | G     | 502 | D5M  | 2       | 0            |
| 2   | P     | 501 | DGT  | 2       | 0            |
| 2   | B     | 501 | DGT  | 1       | 0            |
| 3   | E     | 502 | D5M  | 1       | 0            |
| 2   | K     | 501 | DGT  | 1       | 0            |
| 2   | F     | 501 | DGT  | 2       | 0            |
| 3   | N     | 502 | D5M  | 1       | 0            |
| 3   | C     | 502 | D5M  | 2       | 0            |
| 3   | D     | 502 | D5M  | 2       | 0            |
| 2   | J     | 501 | DGT  | 3       | 0            |
| 3   | J     | 502 | D5M  | 1       | 0            |
| 3   | M     | 502 | D5M  | 1       | 0            |
| 2   | D     | 501 | DGT  | 3       | 0            |
| 3   | L     | 502 | D5M  | 1       | 0            |
| 3   | K     | 502 | D5M  | 2       | 0            |
| 3   | B     | 502 | D5M  | 1       | 0            |
| 3   | P     | 502 | D5M  | 2       | 0            |
| 2   | A     | 501 | DGT  | 2       | 0            |
| 3   | F     | 502 | D5M  | 1       | 0            |

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

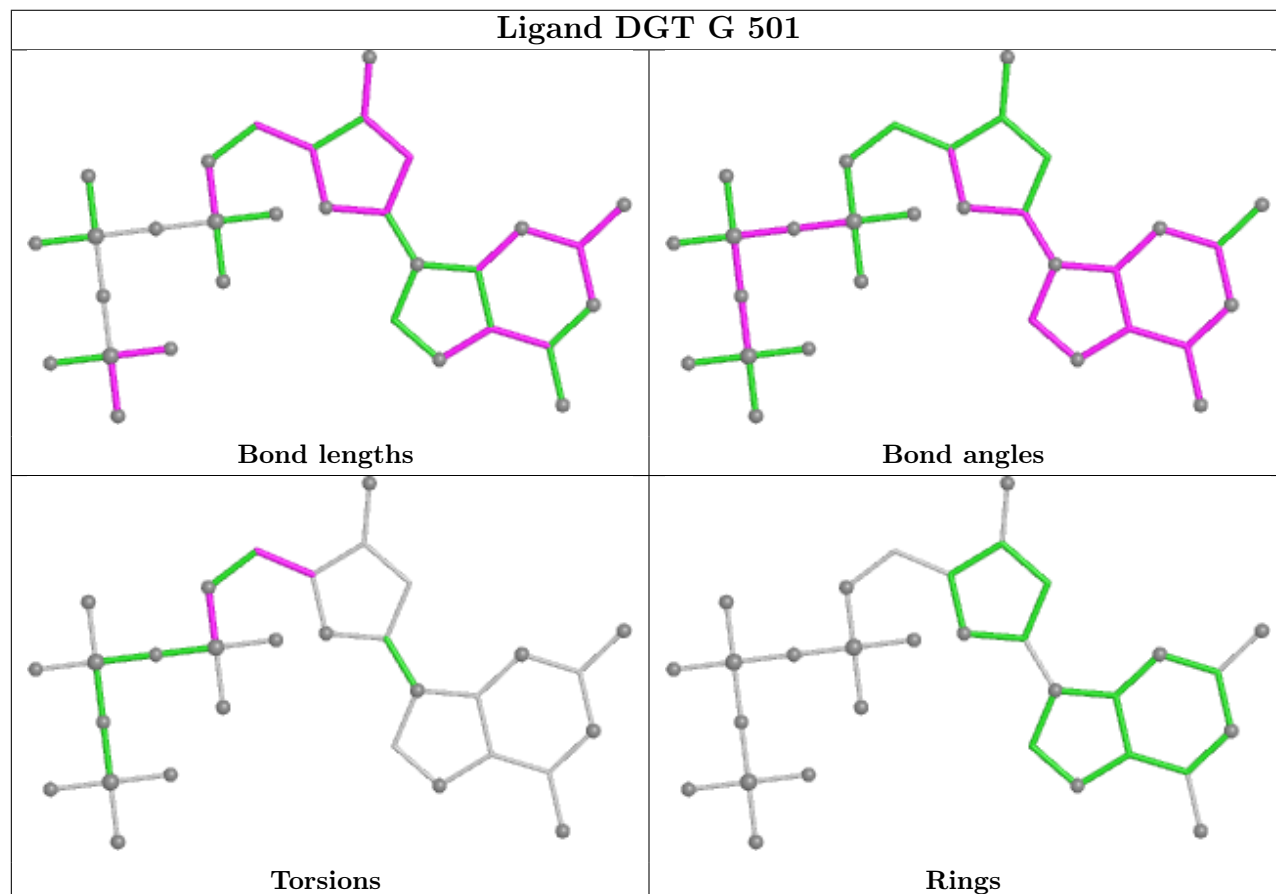
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

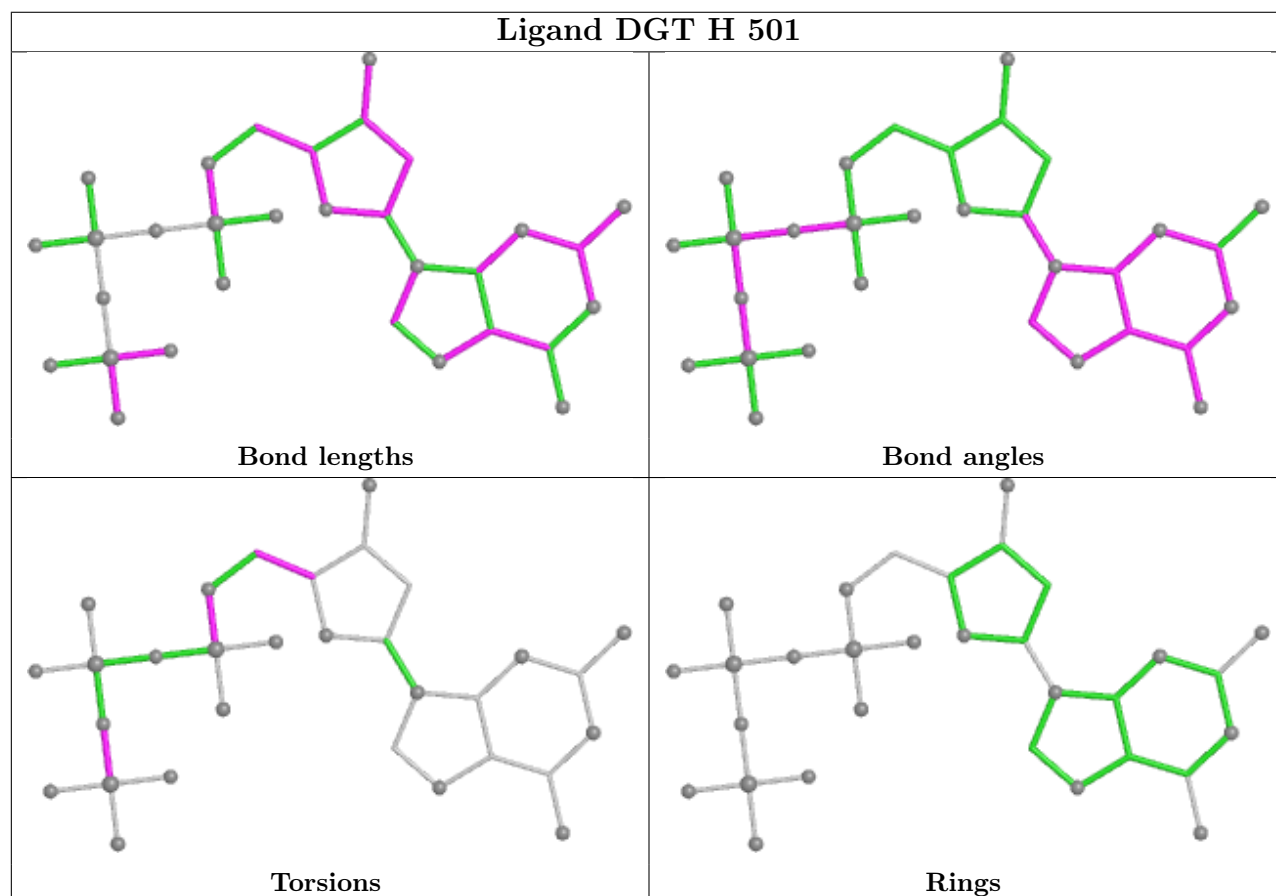
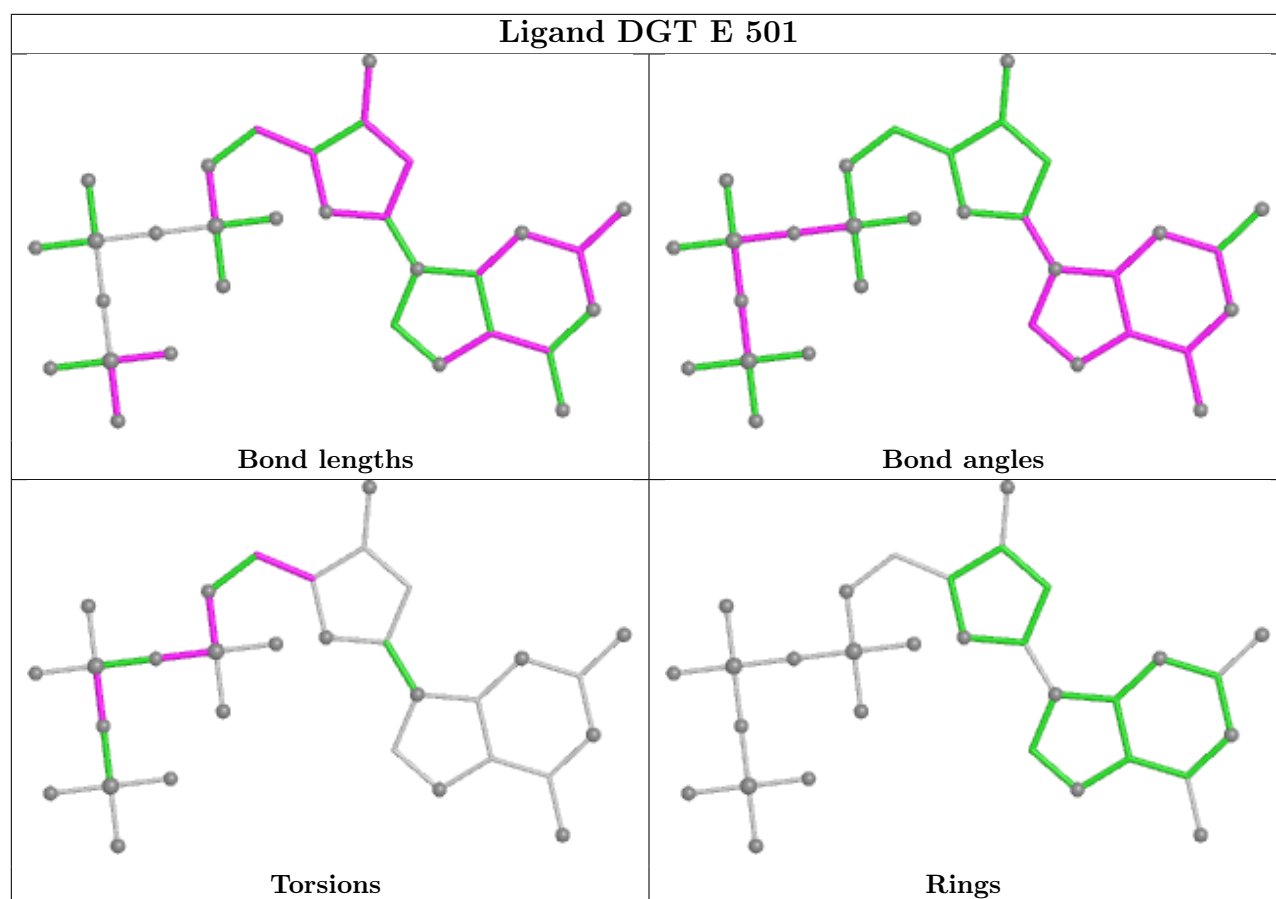


## Ligand DGT L 501

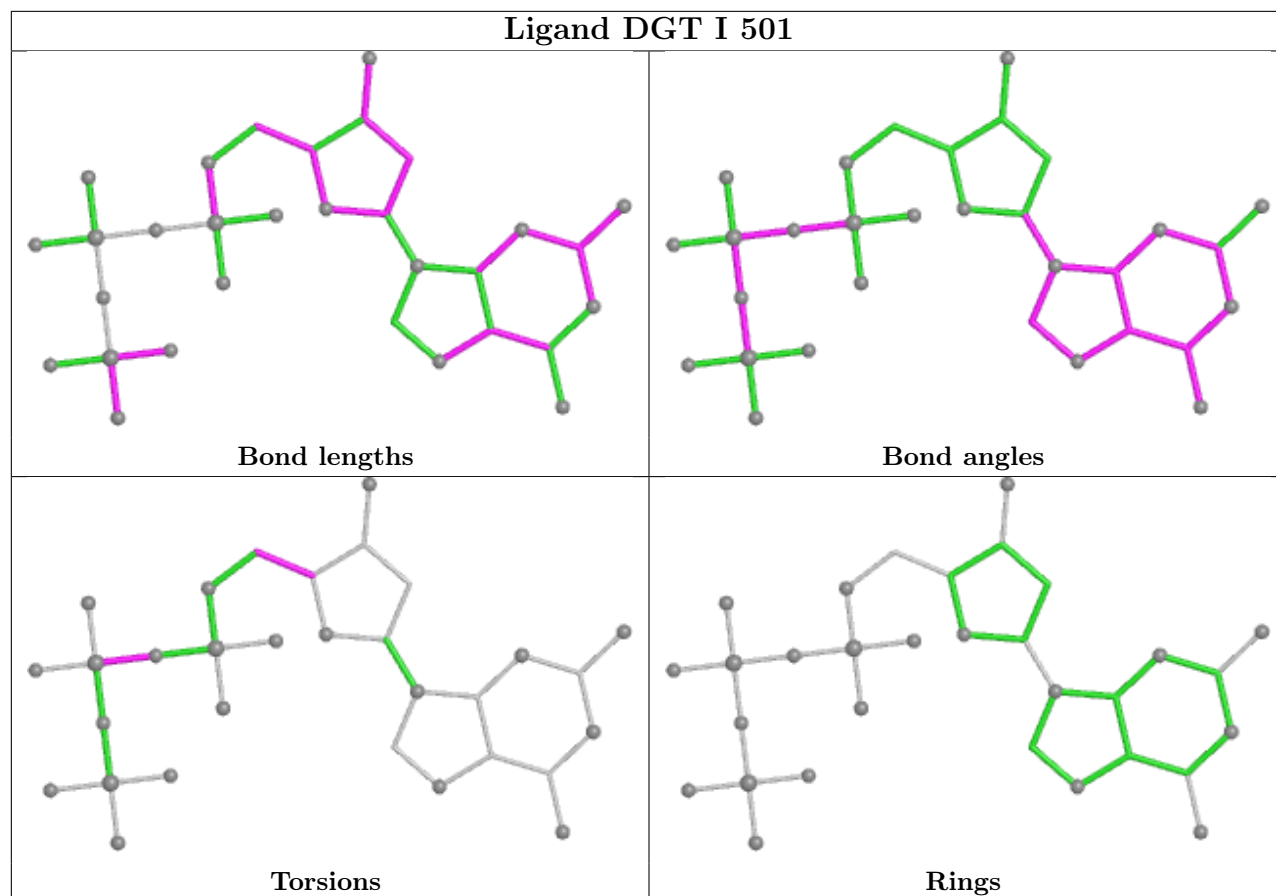


## Ligand DGT G 501

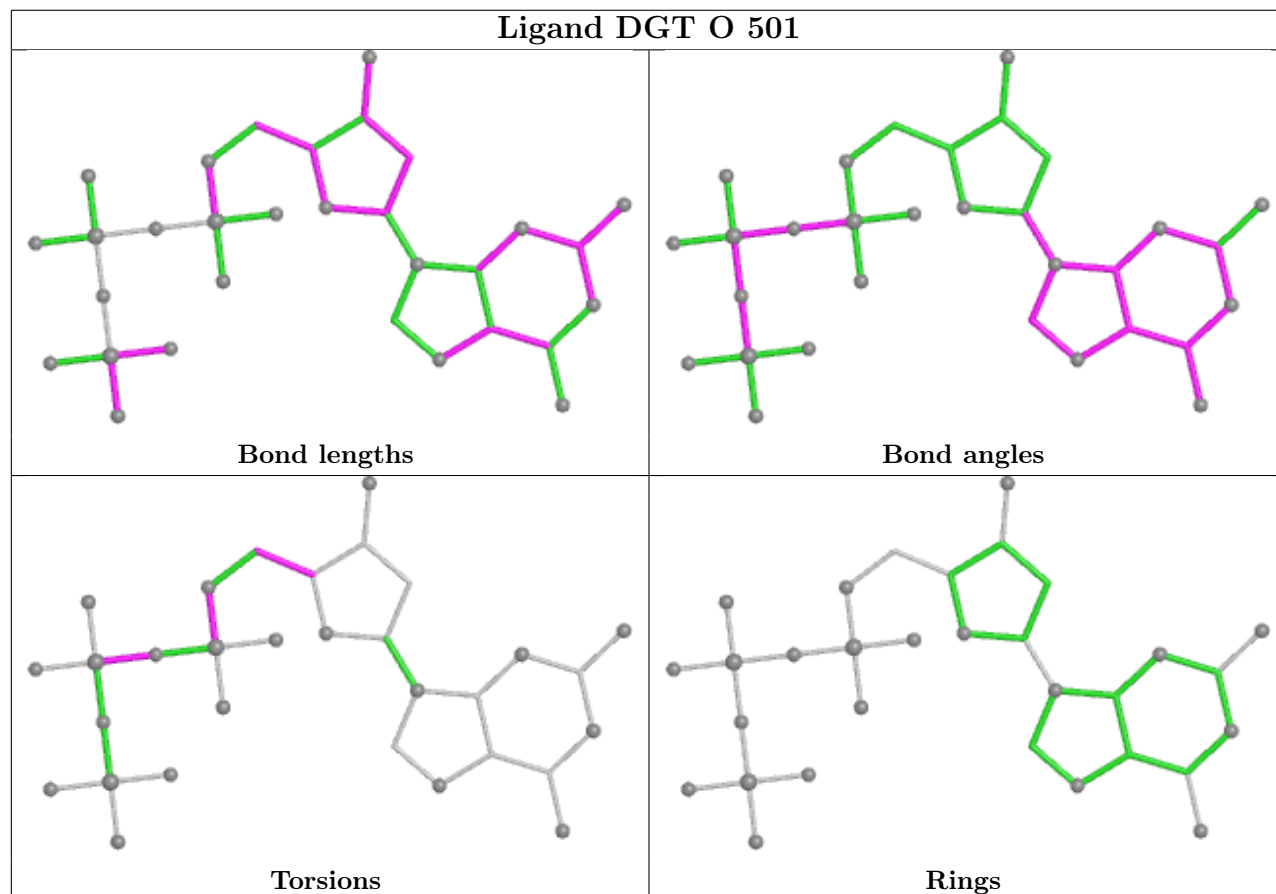




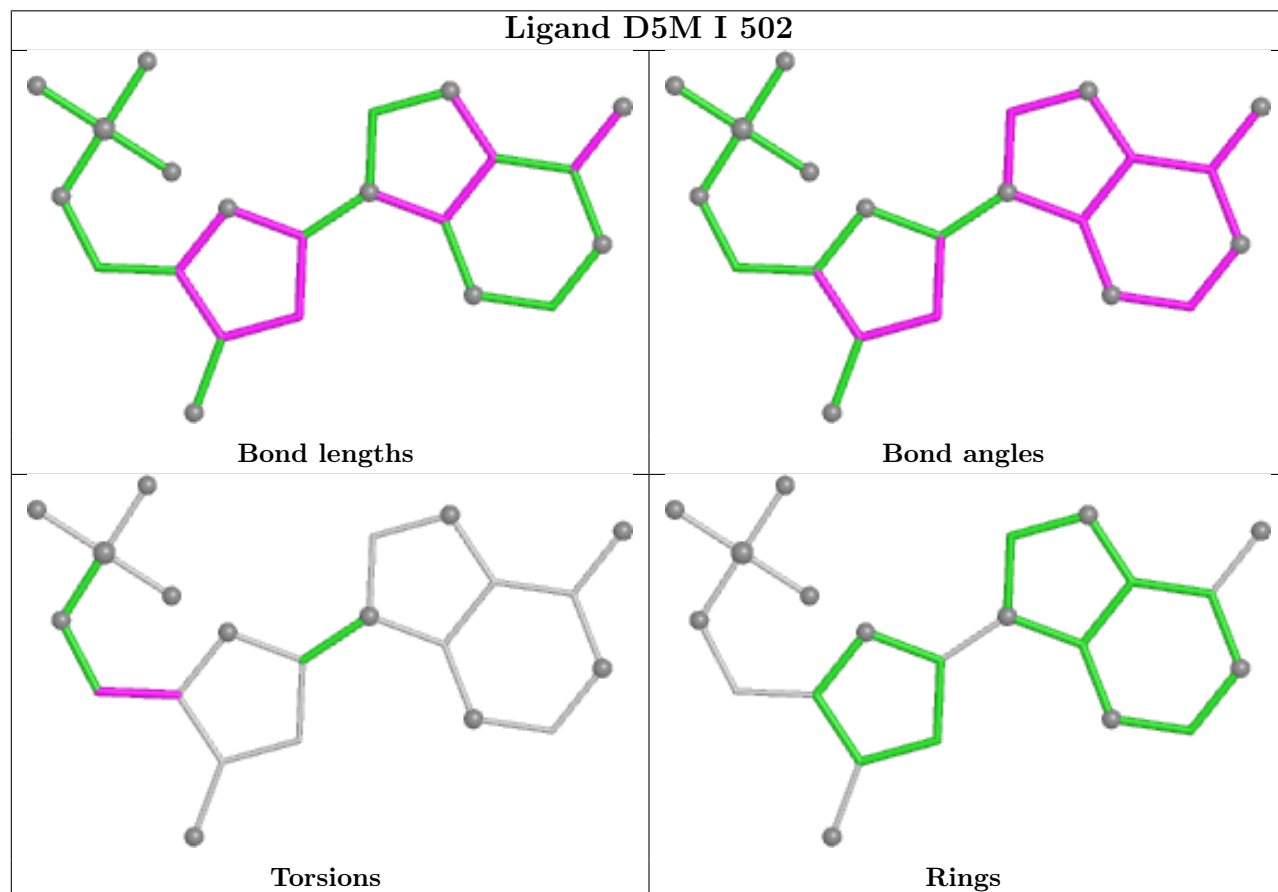
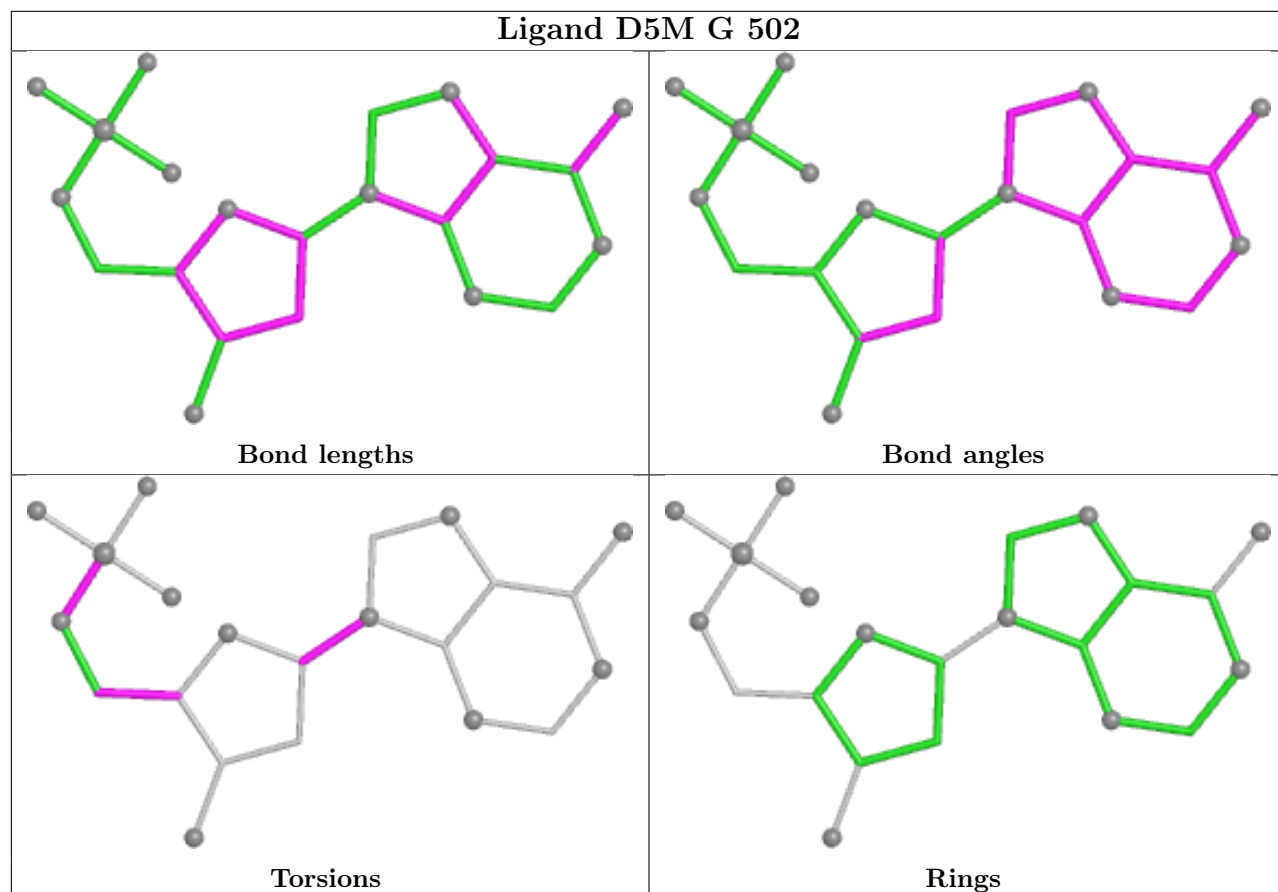
## Ligand DGT I 501

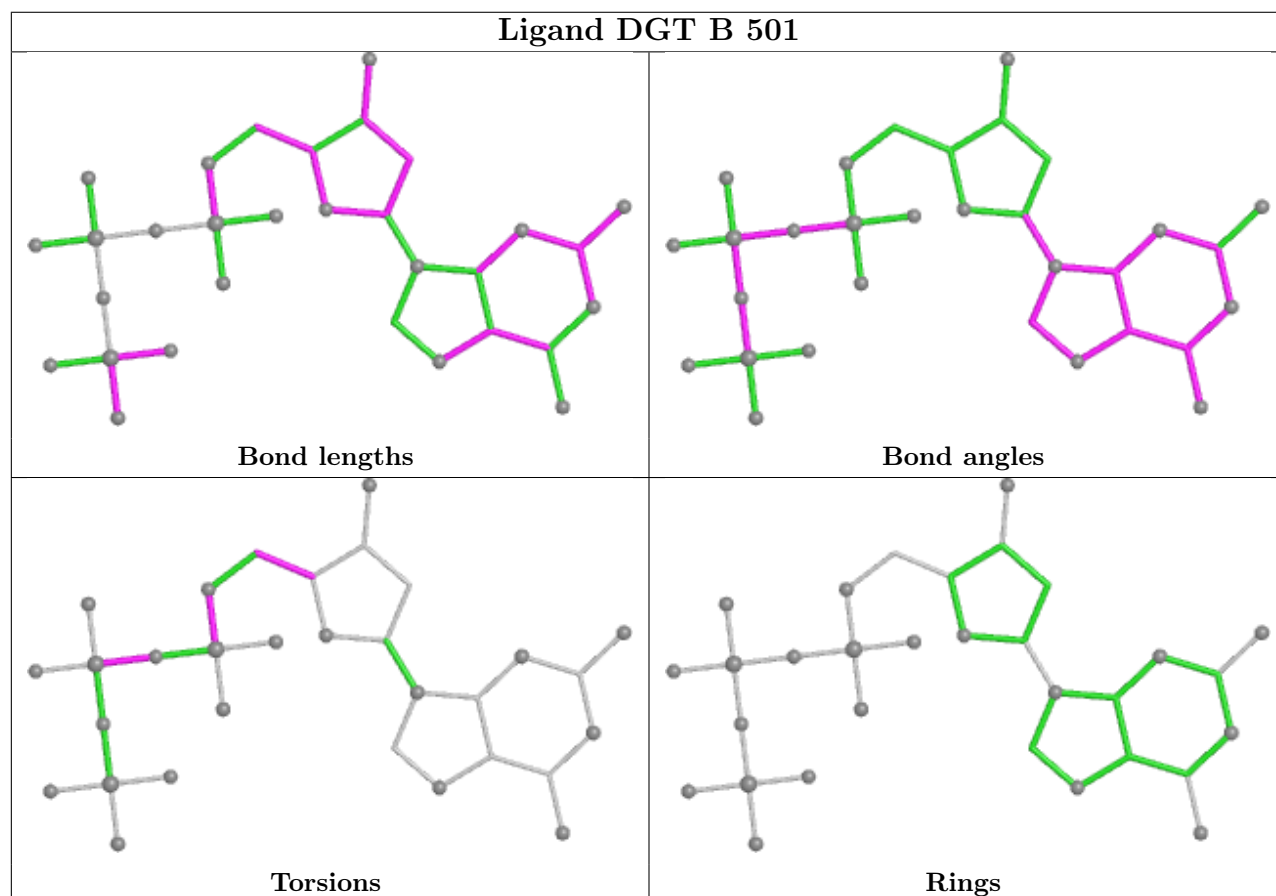
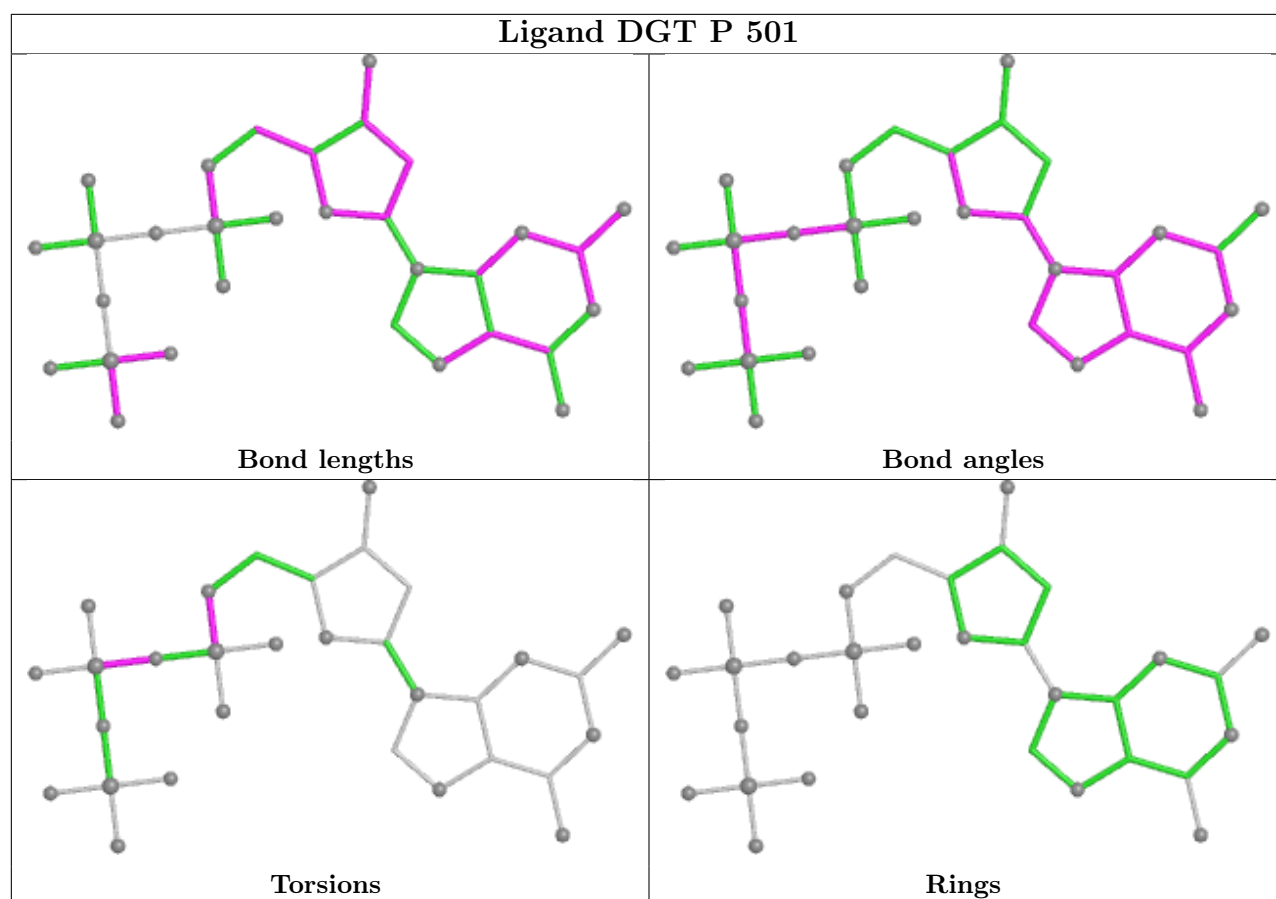


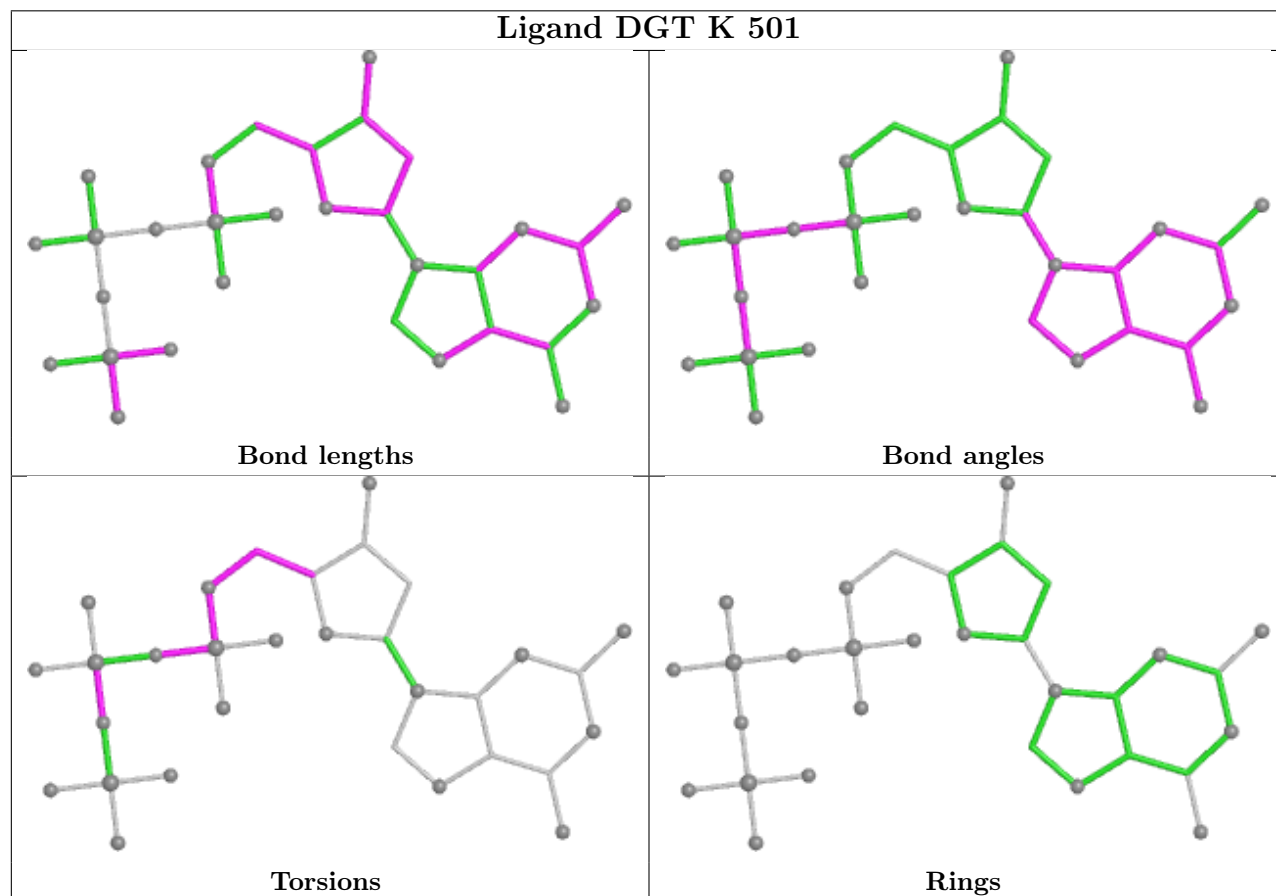
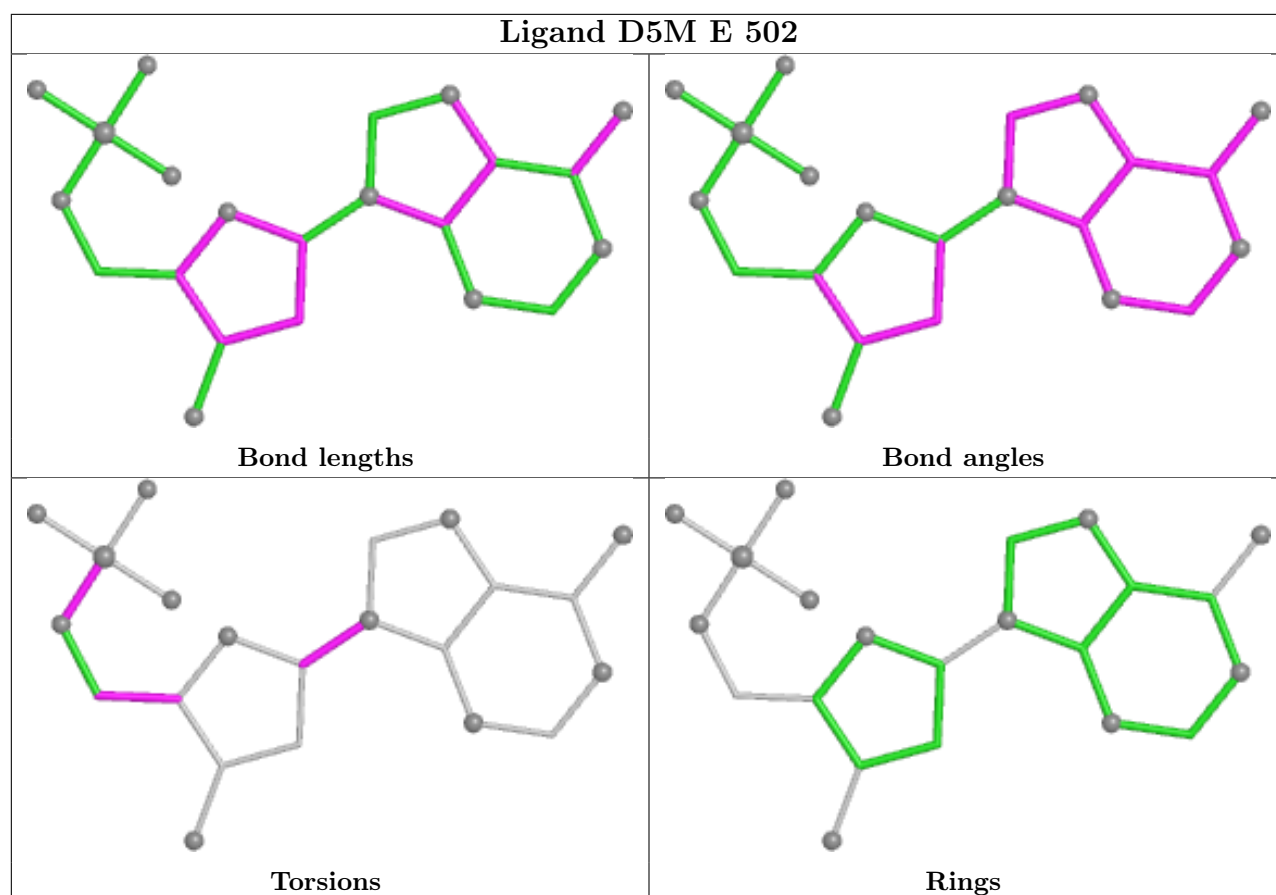
## Ligand DGT O 501

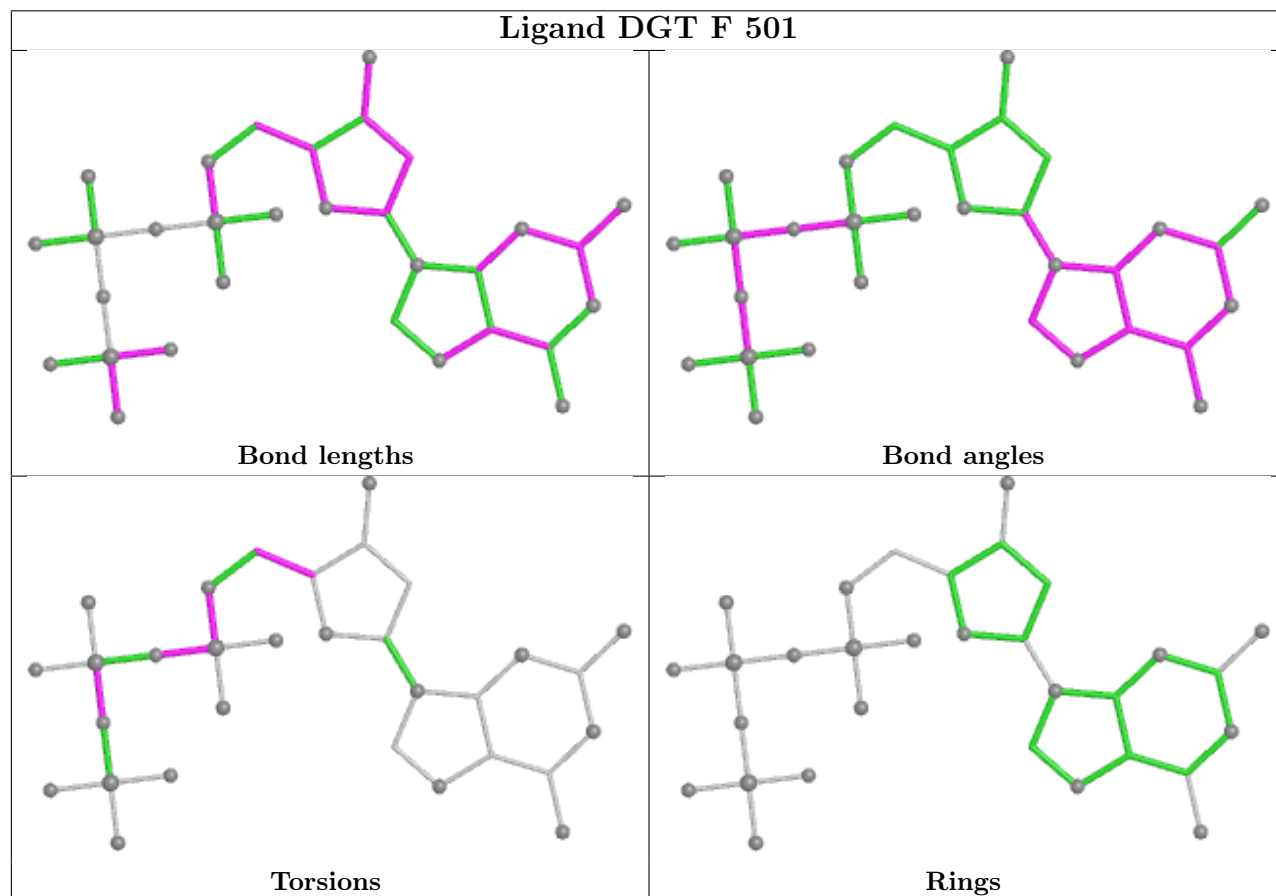
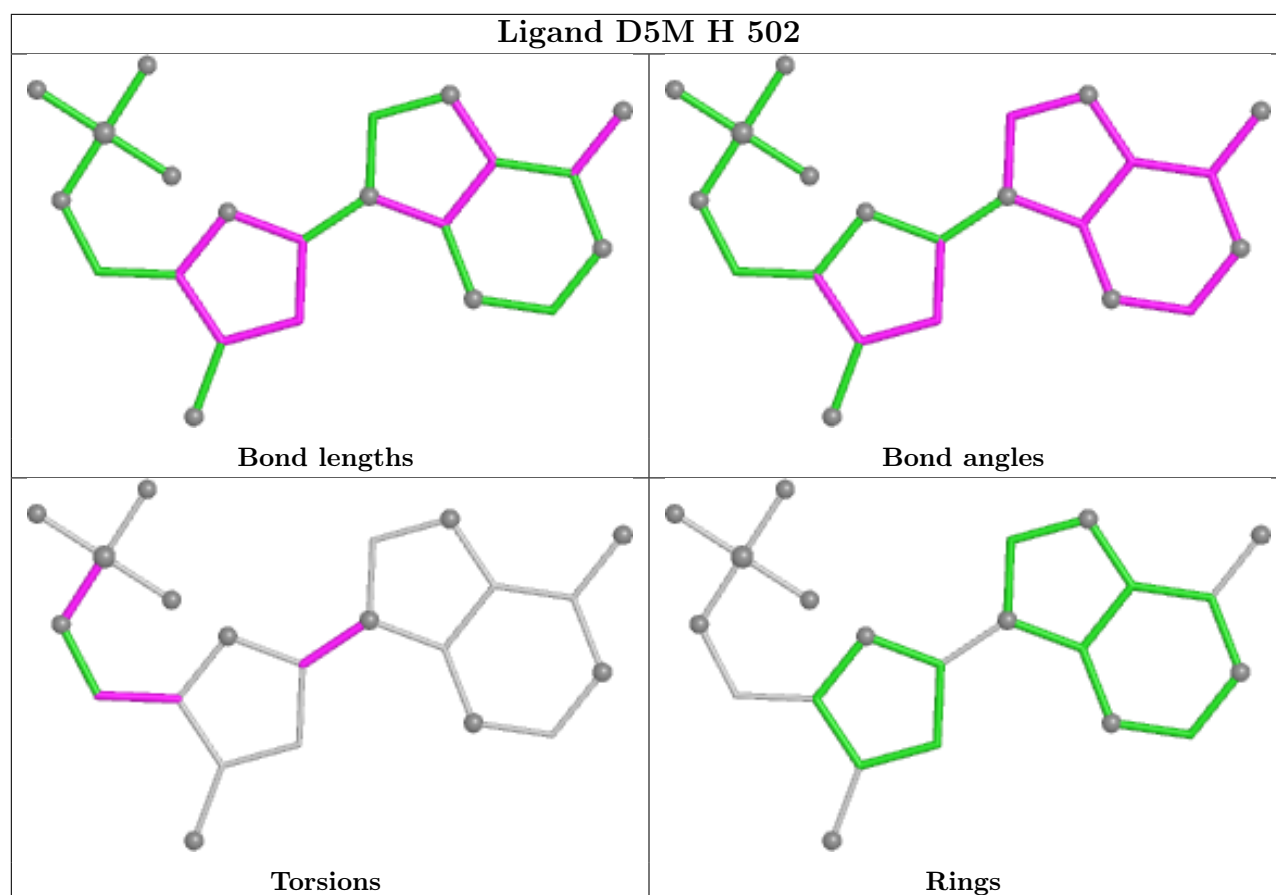


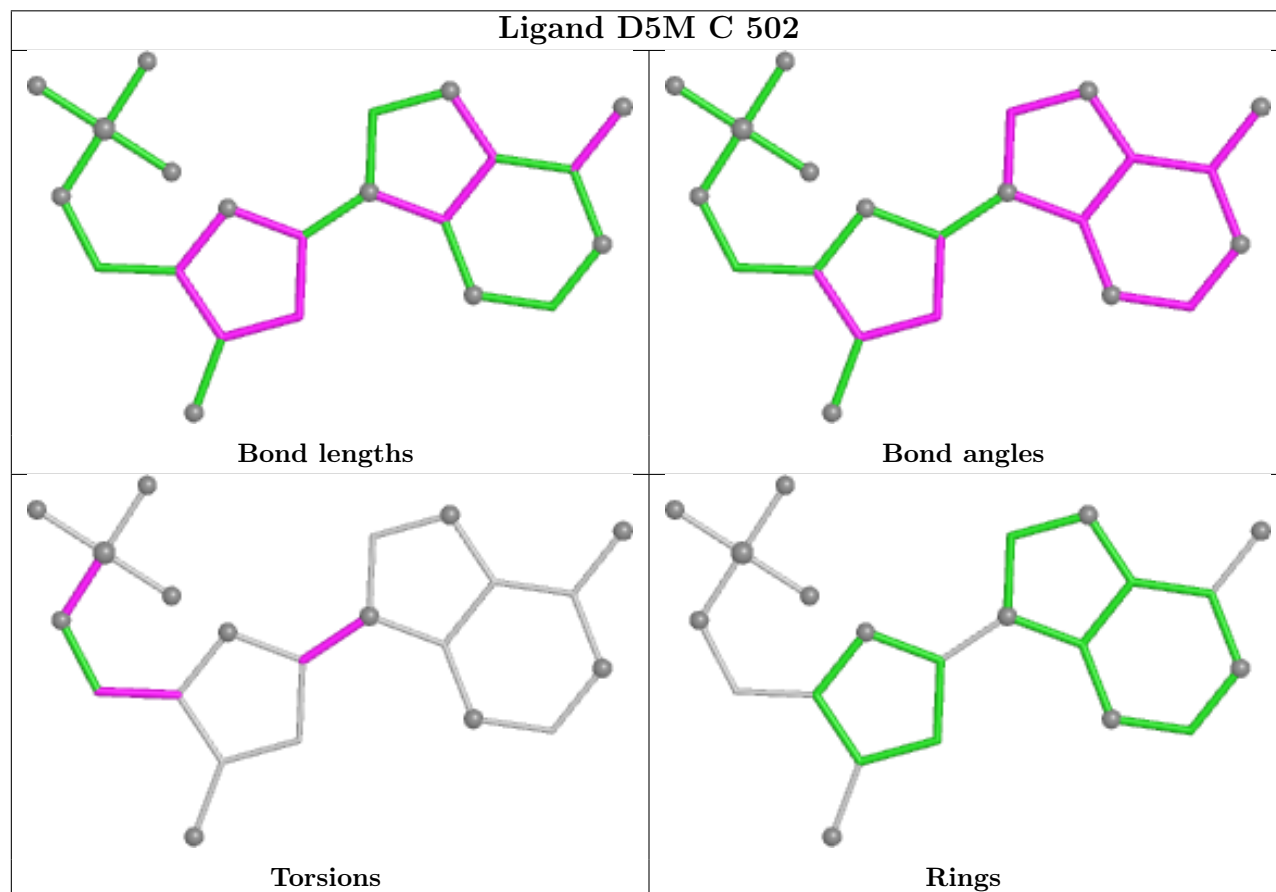
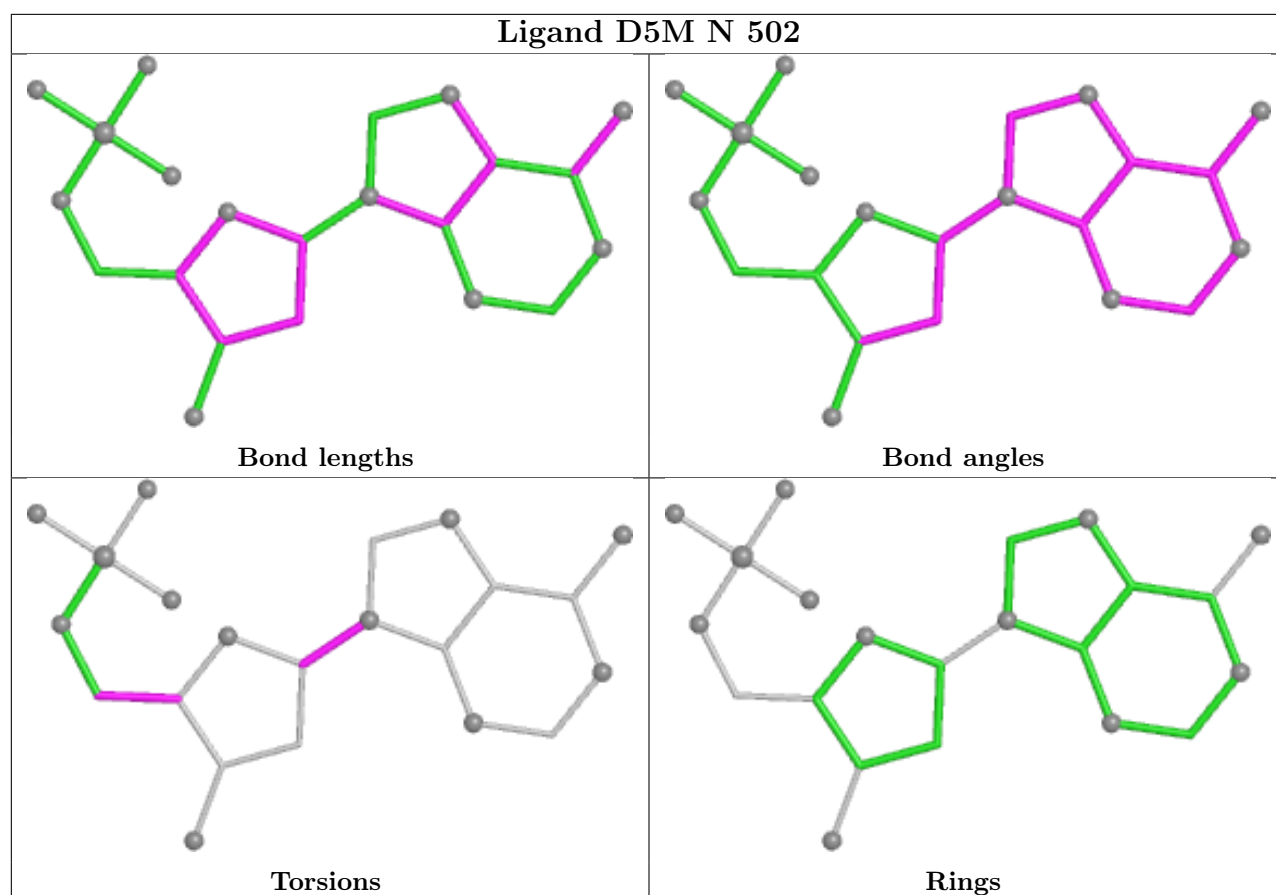


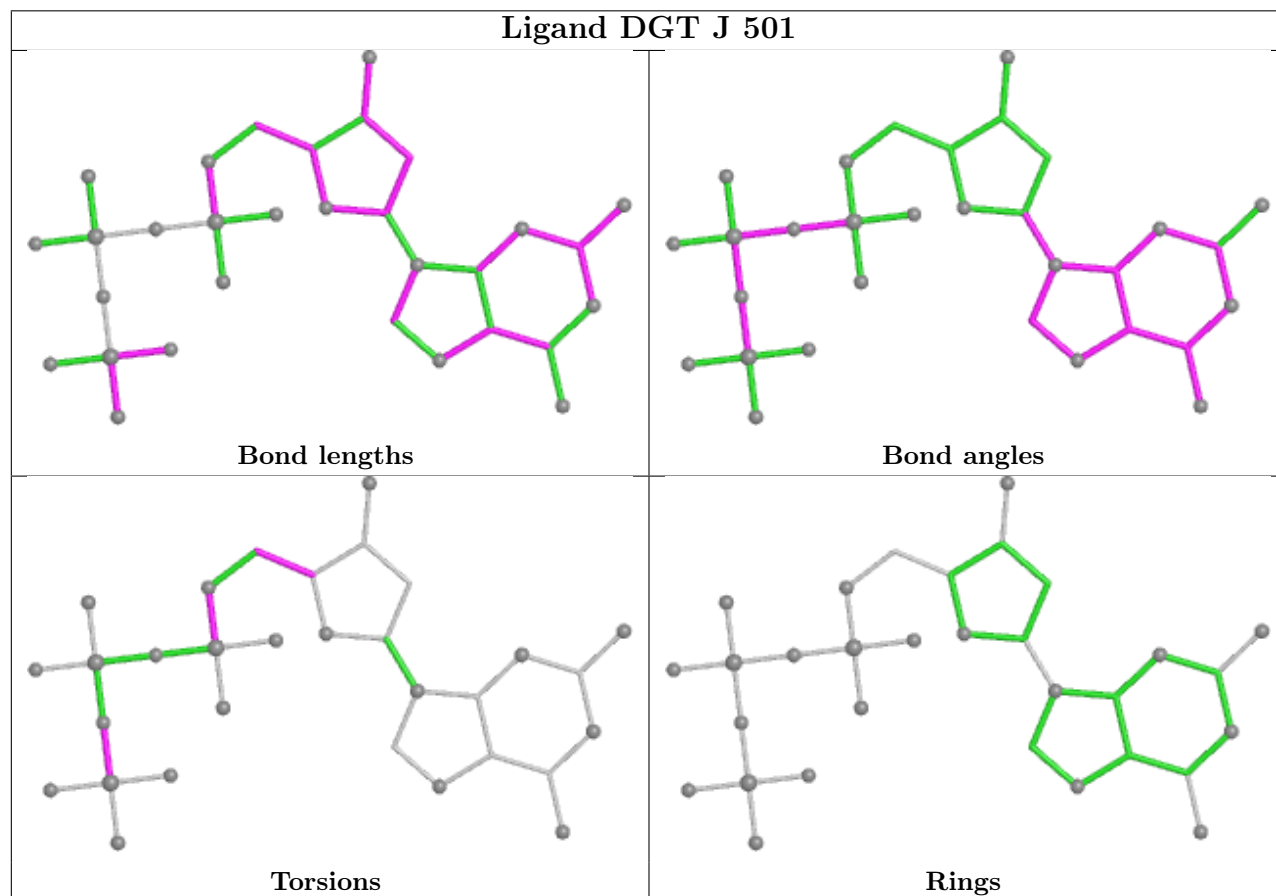
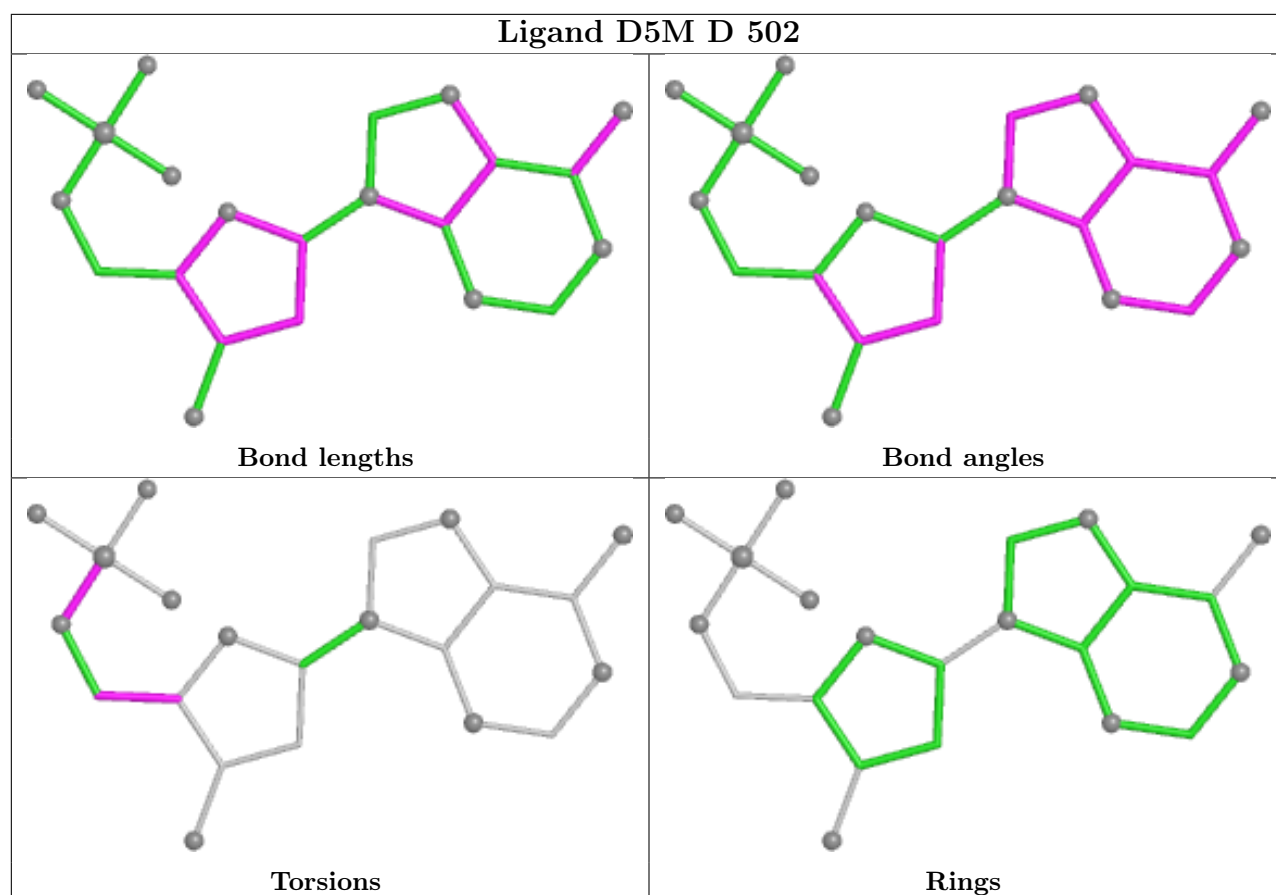


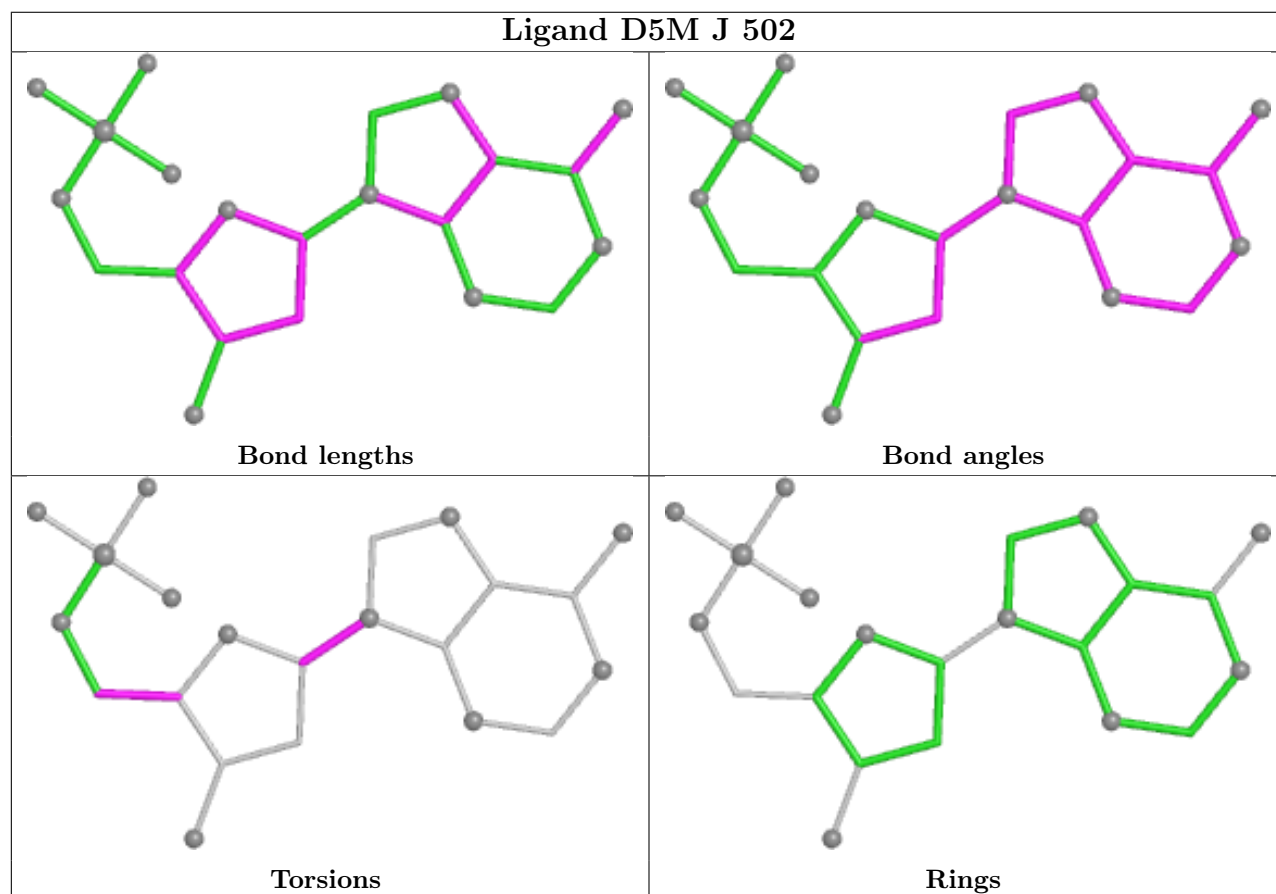
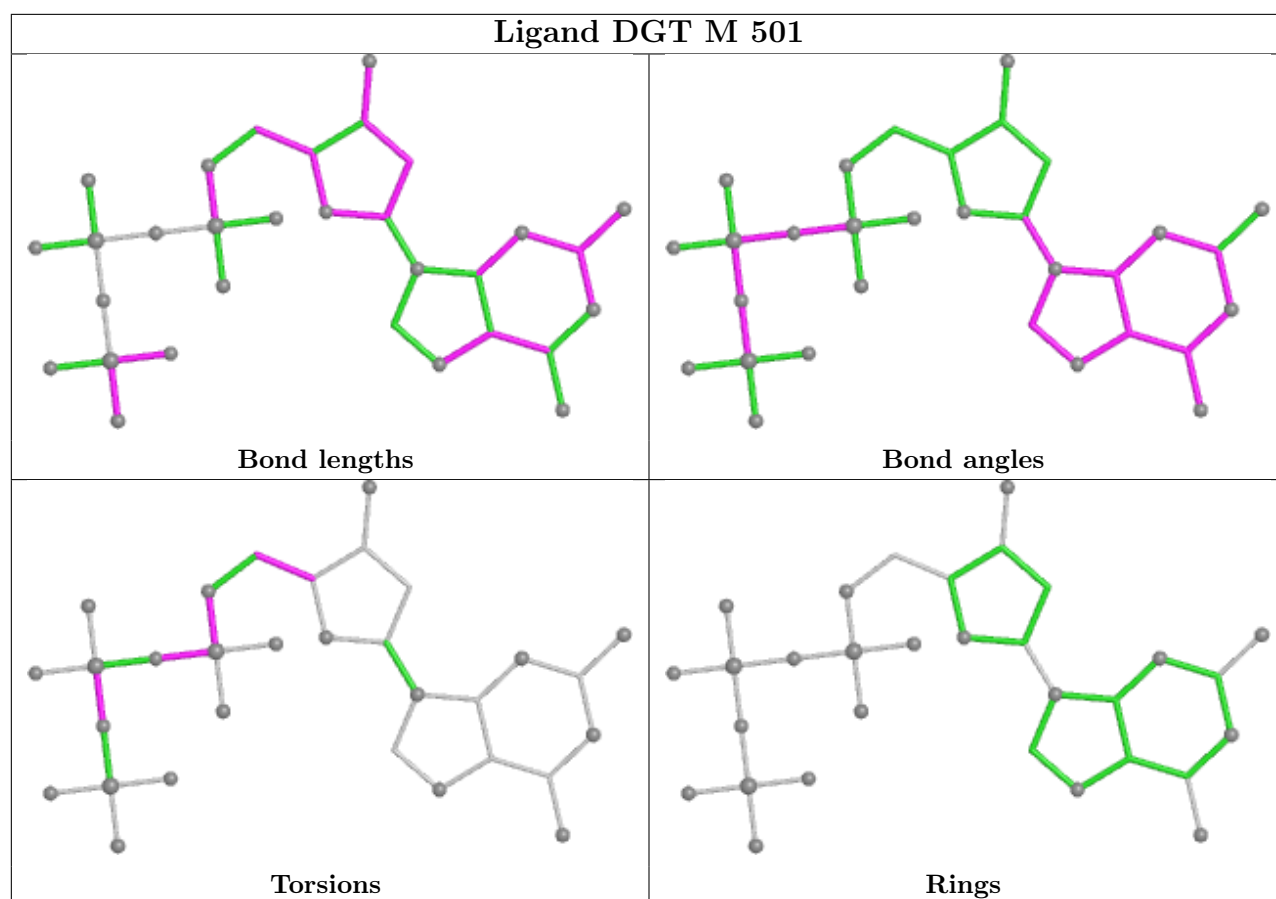


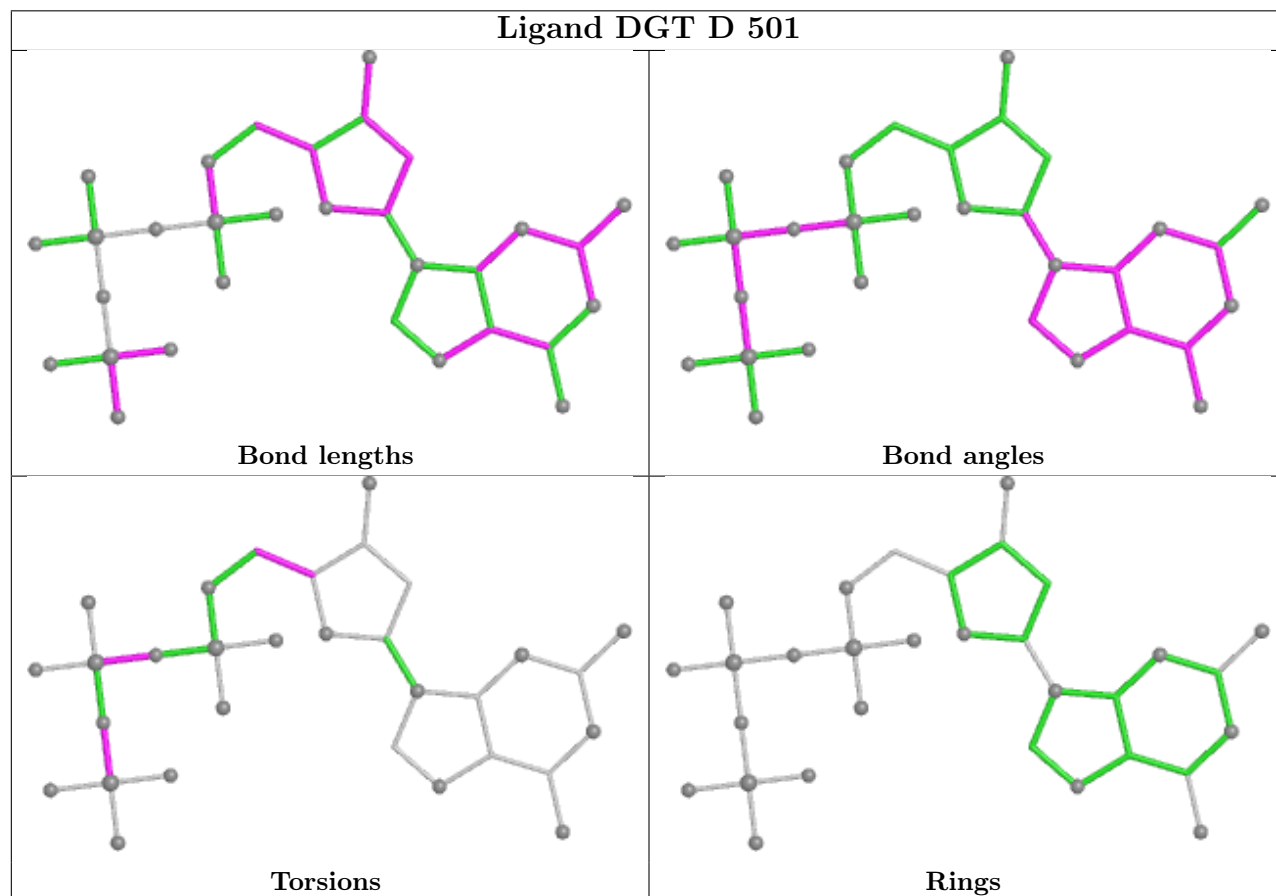
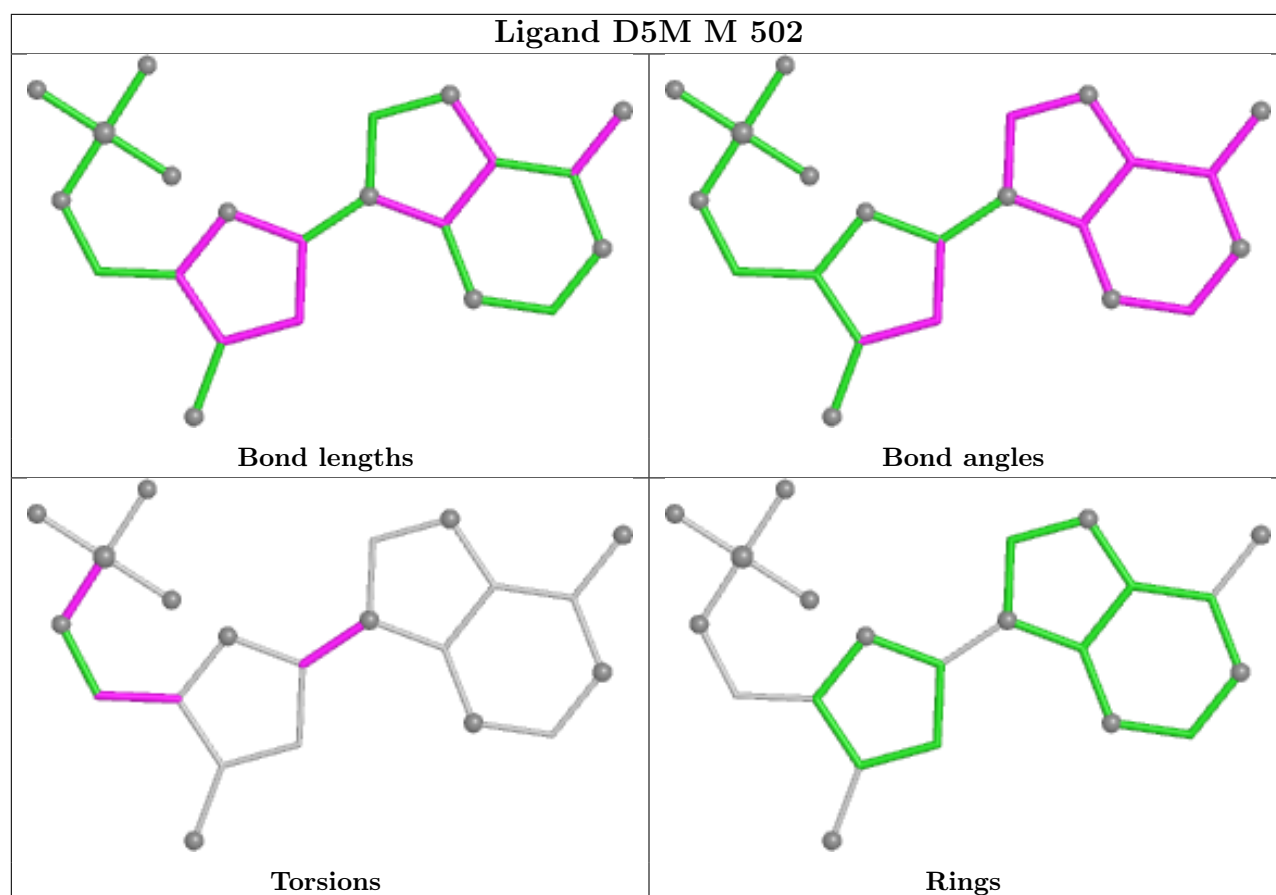




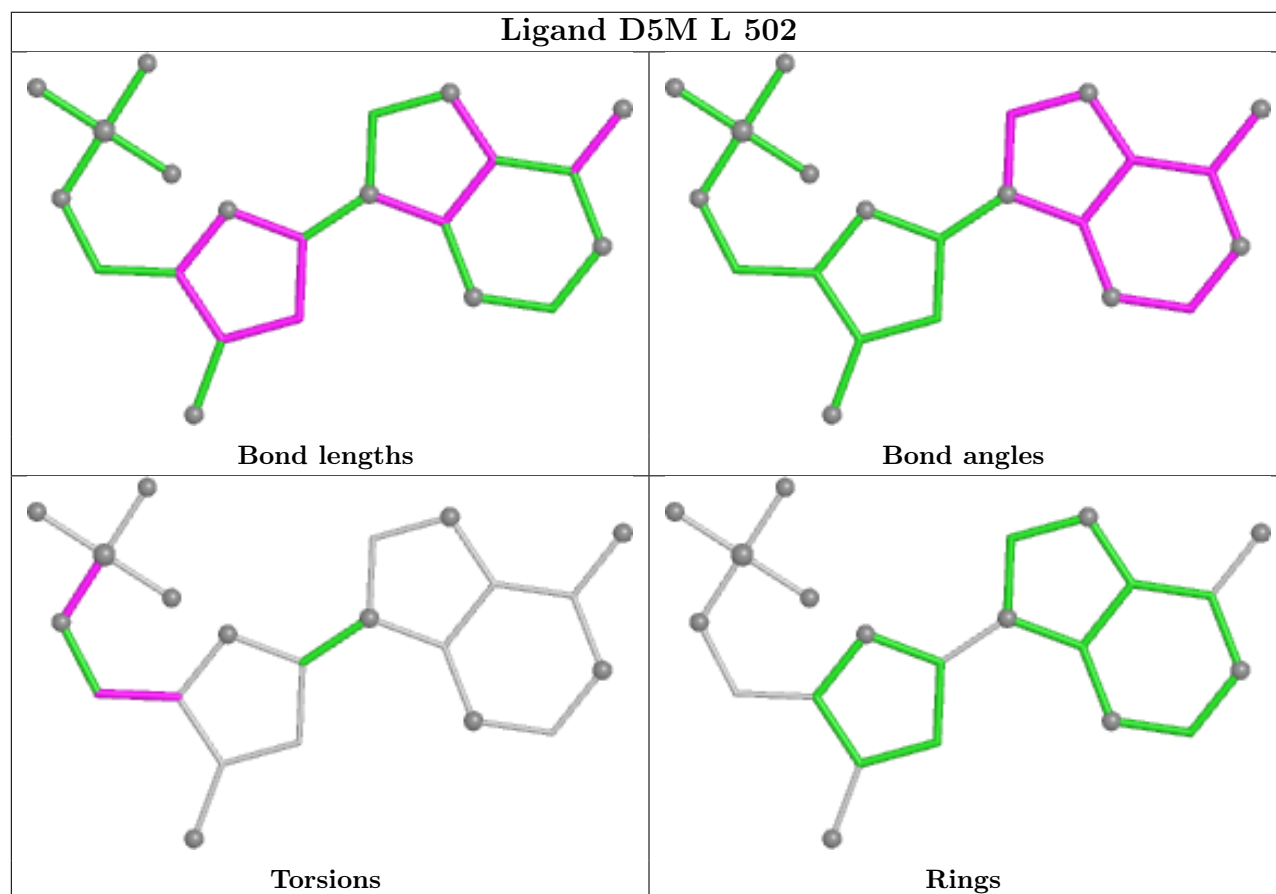
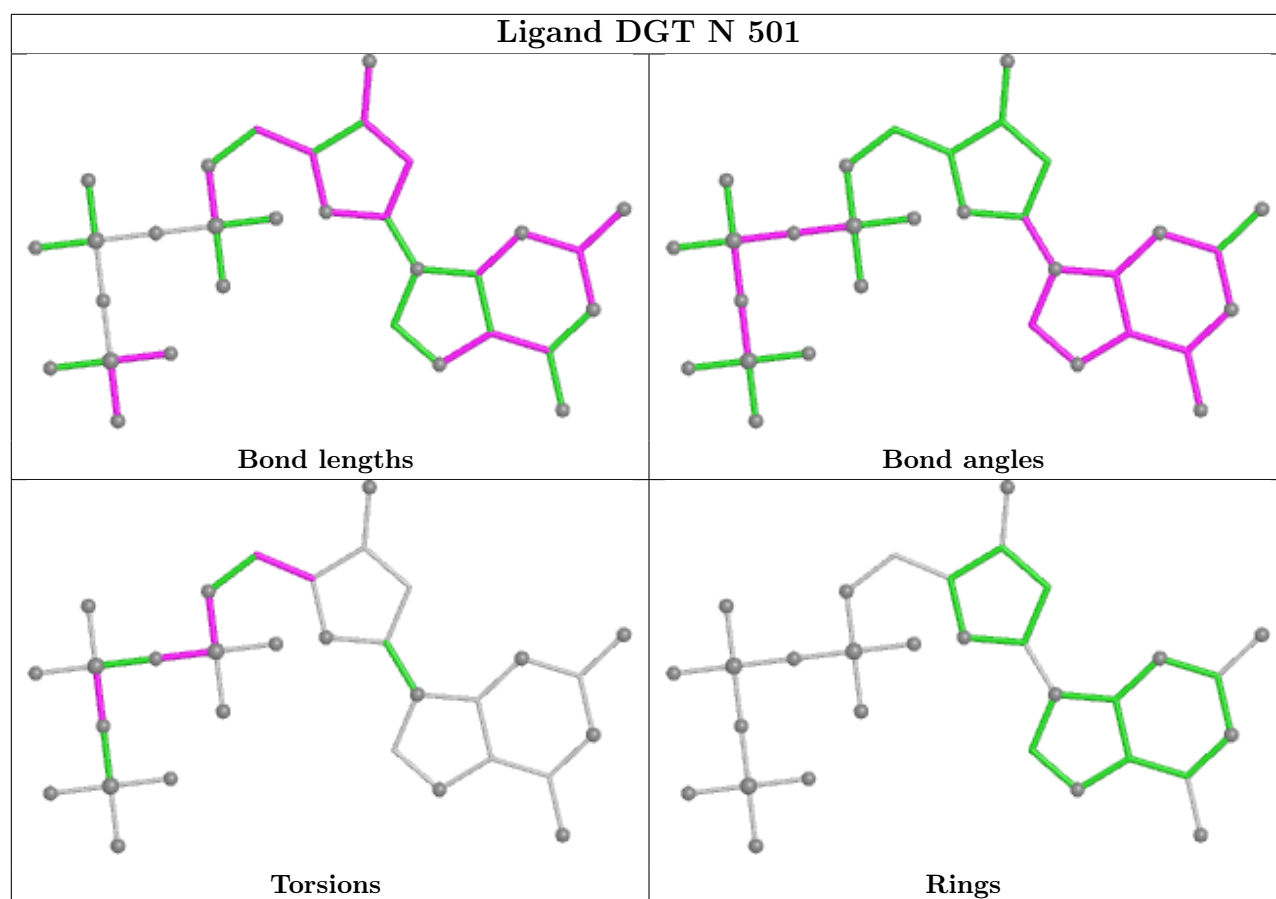


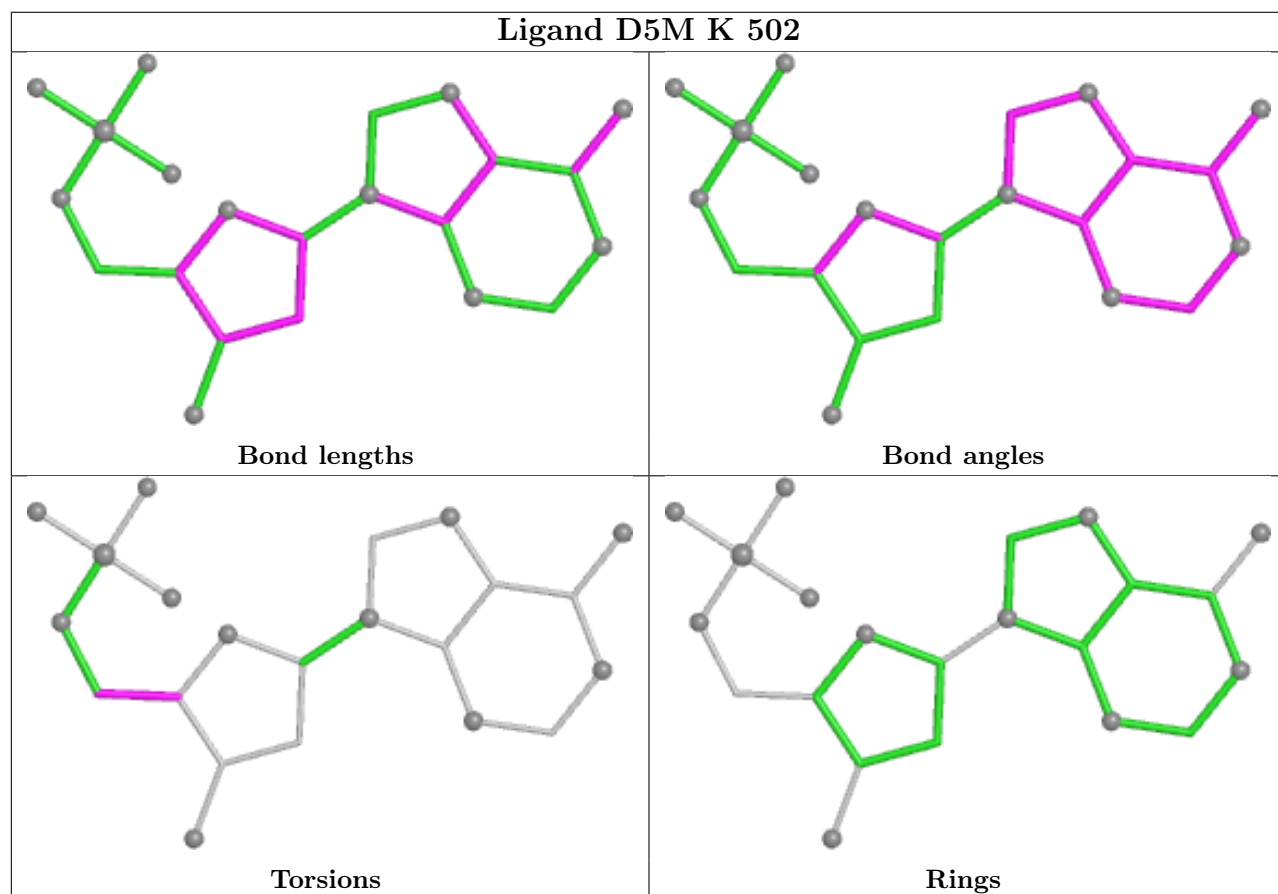
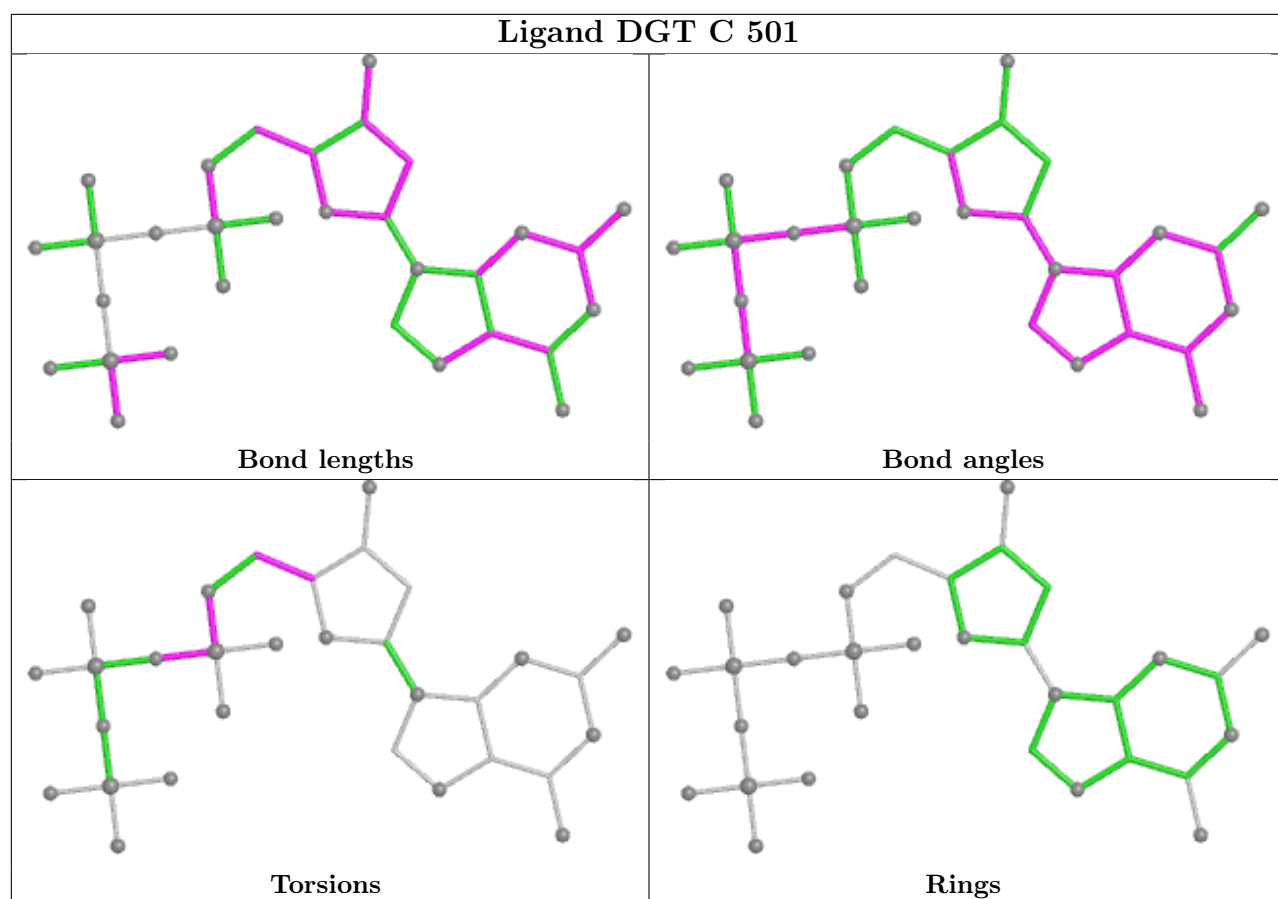


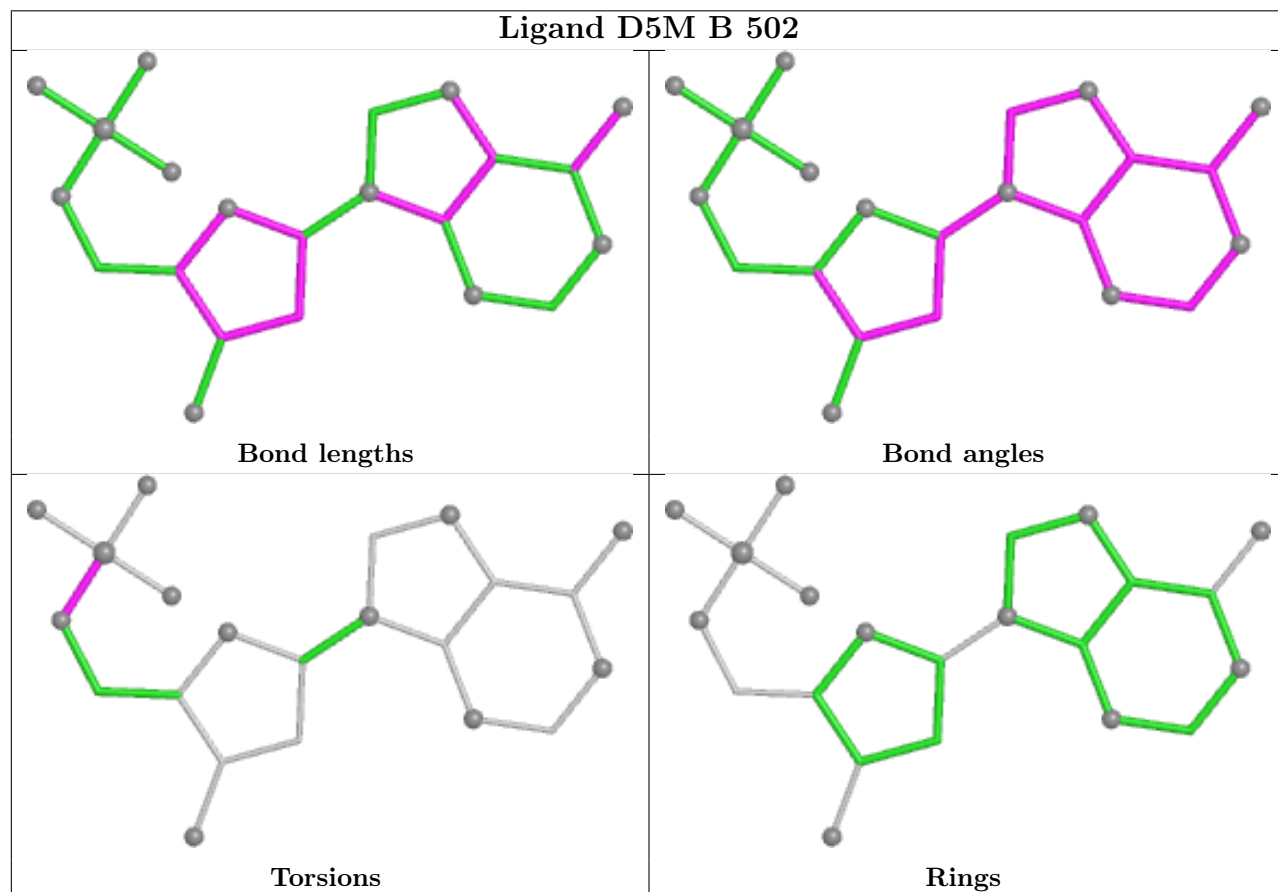
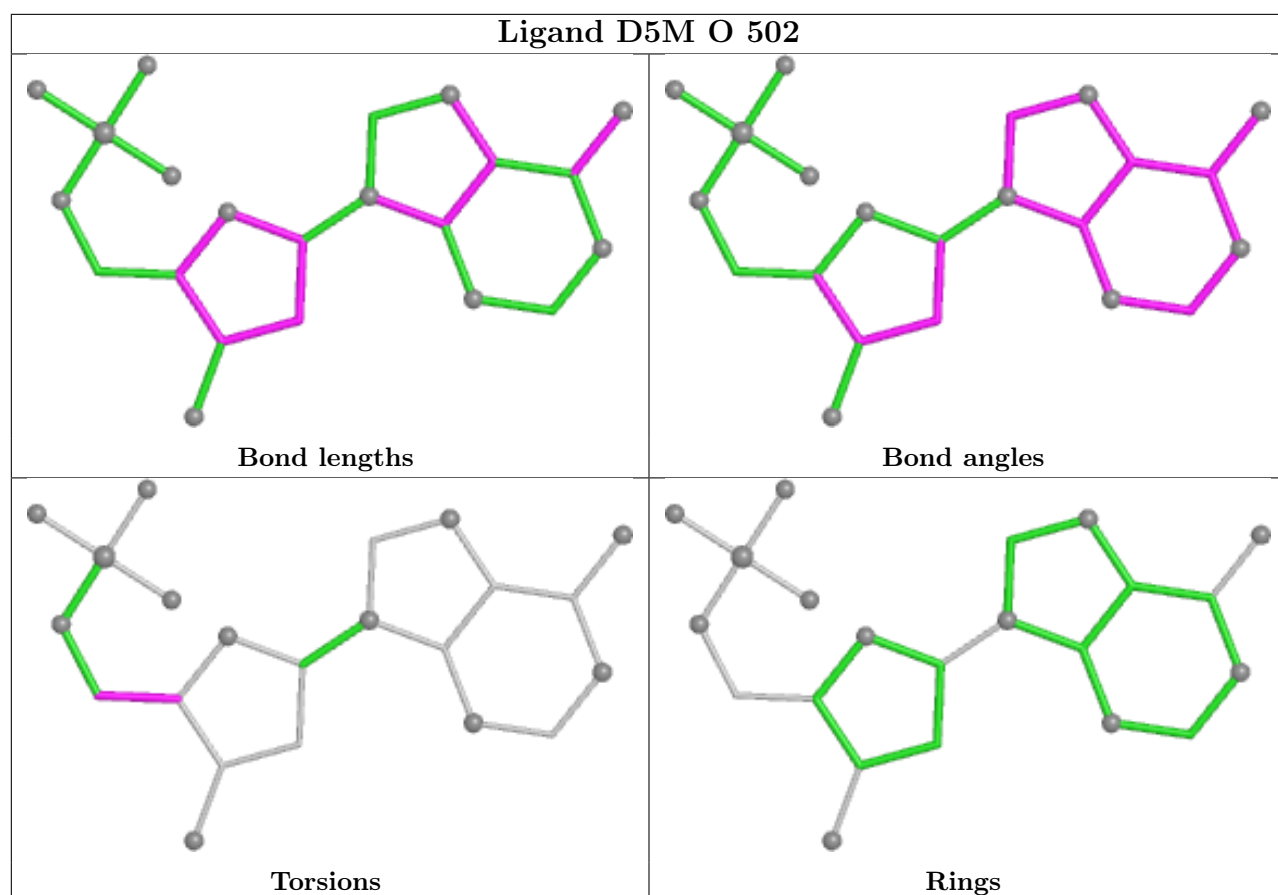


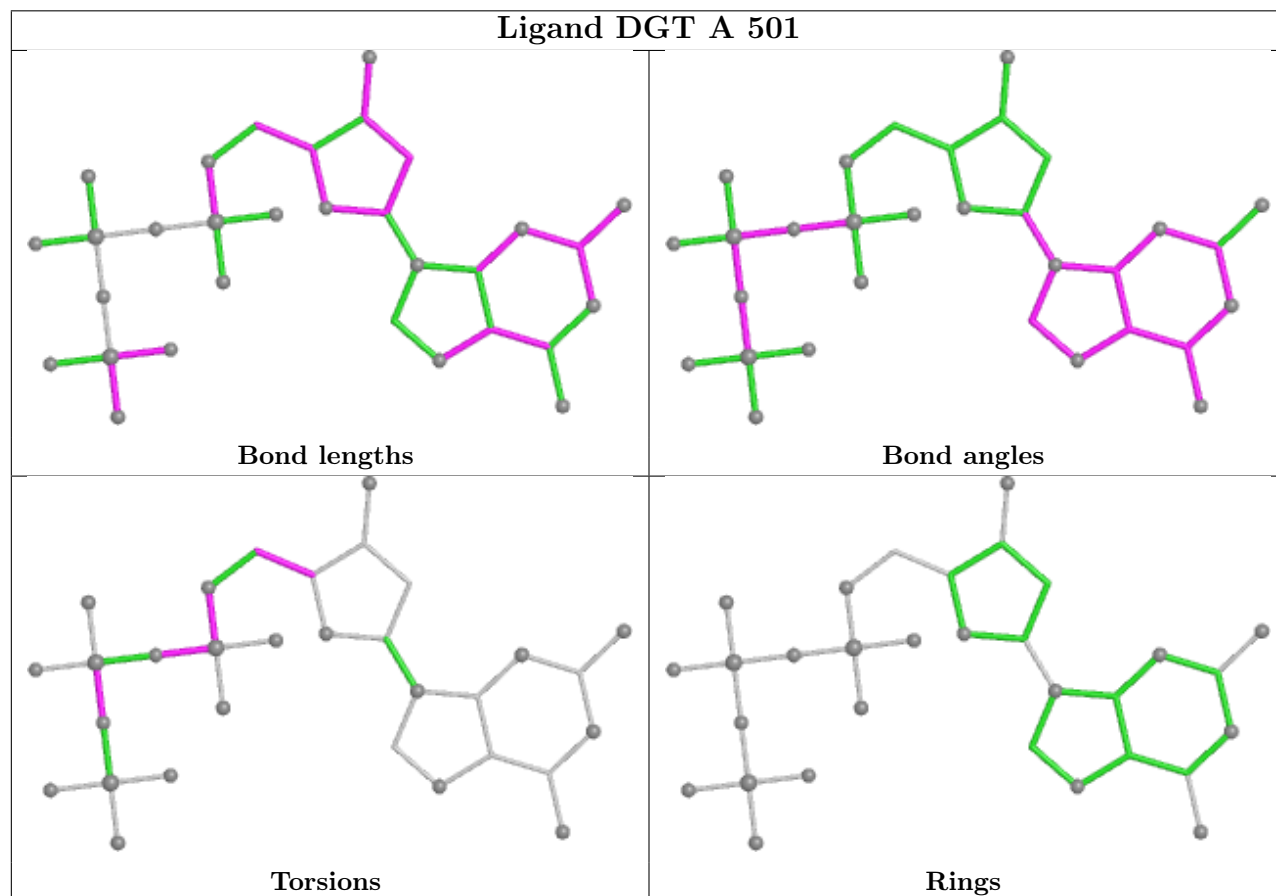
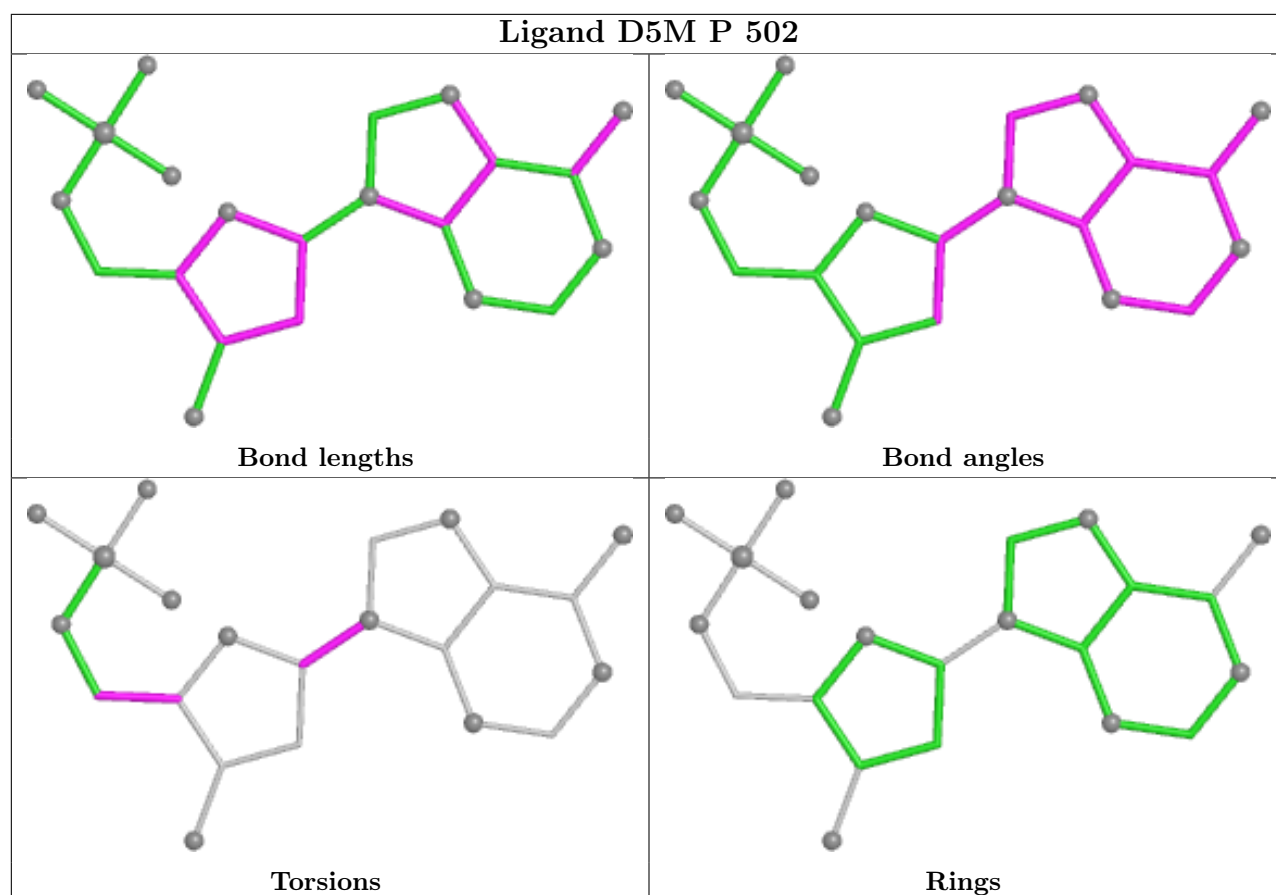


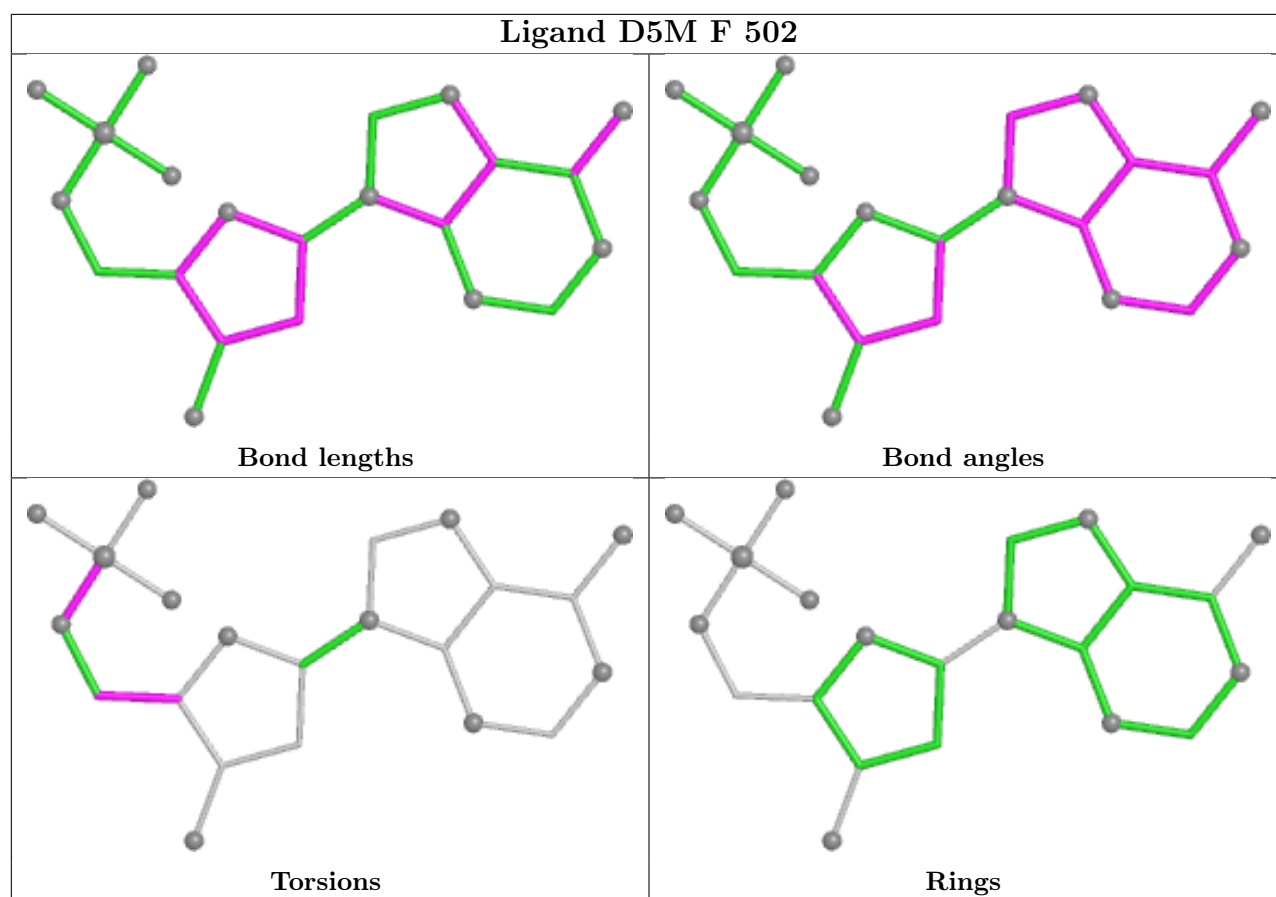












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

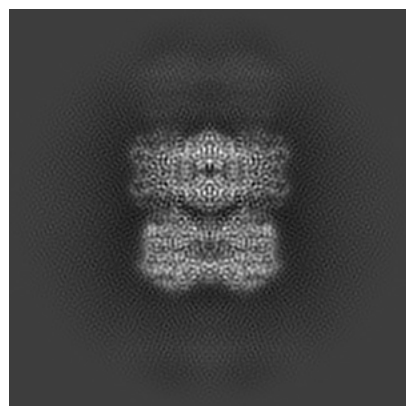
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65396. These allow visual inspection of the internal detail of the map and identification of artifacts.

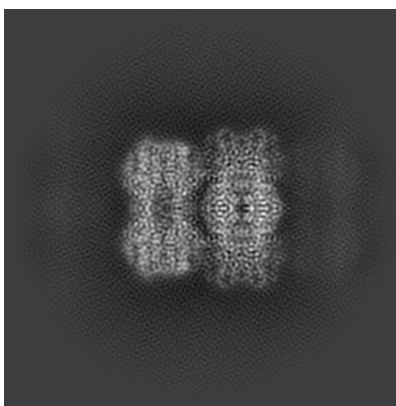
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

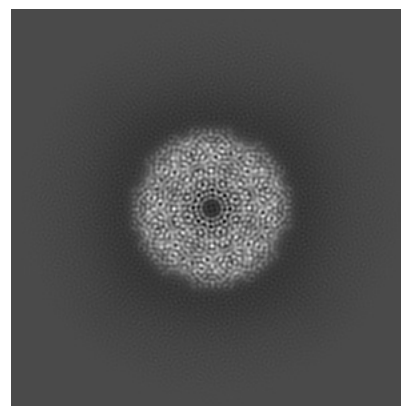
#### 6.1.1 Primary map



X

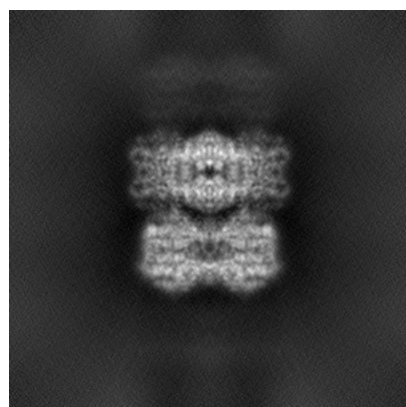


Y

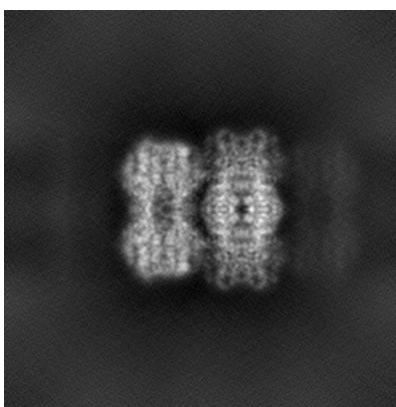


Z

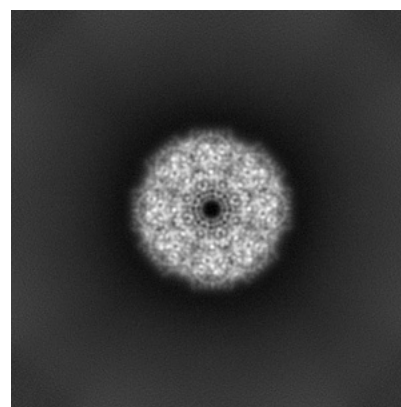
#### 6.1.2 Raw map



X



Y

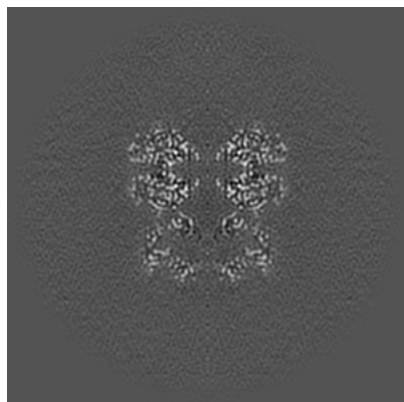


Z

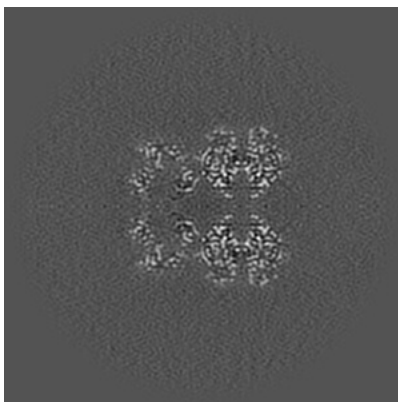
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

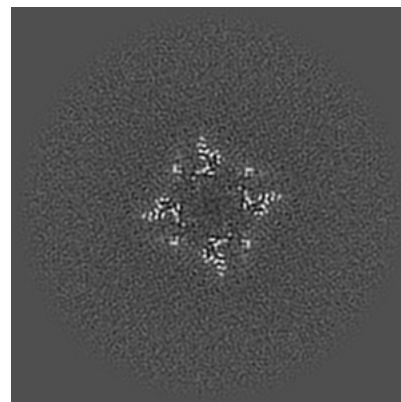
### 6.2.1 Primary map



X Index: 160

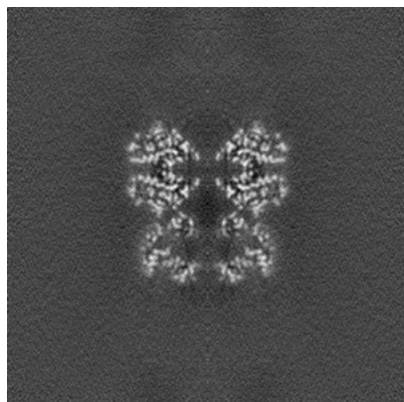


Y Index: 160

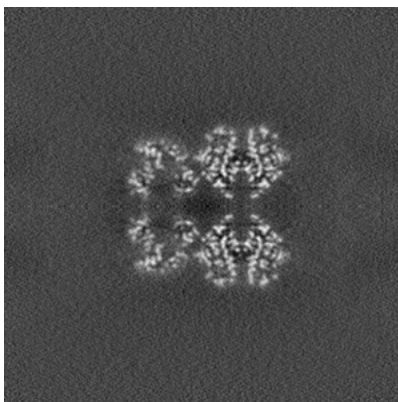


Z Index: 160

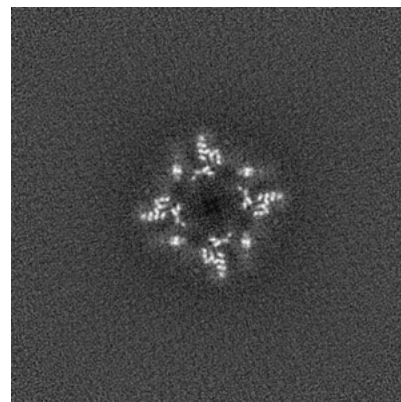
### 6.2.2 Raw map



X Index: 160



Y Index: 160



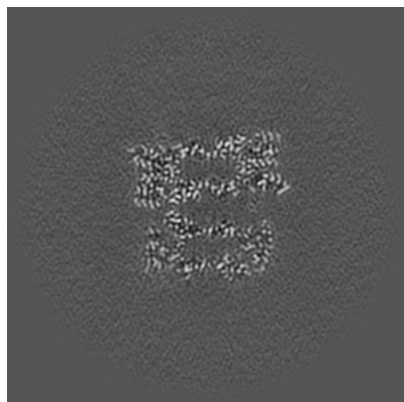
Z Index: 160

The images above show central slices of the map in three orthogonal directions.

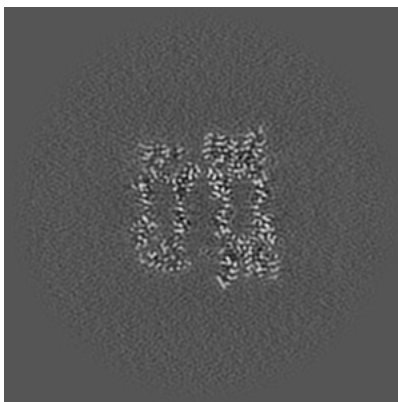


## 6.3 Largest variance slices [i](#)

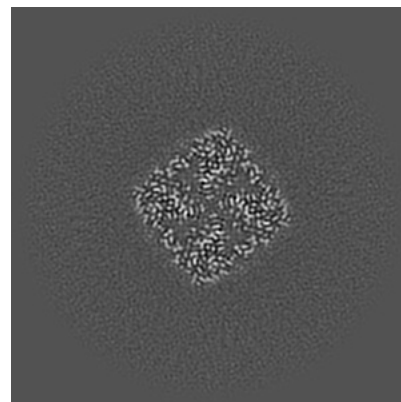
### 6.3.1 Primary map



X Index: 169

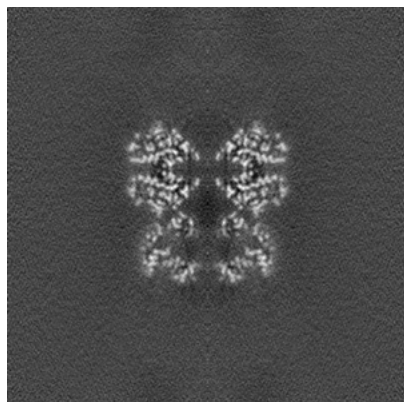


Y Index: 169

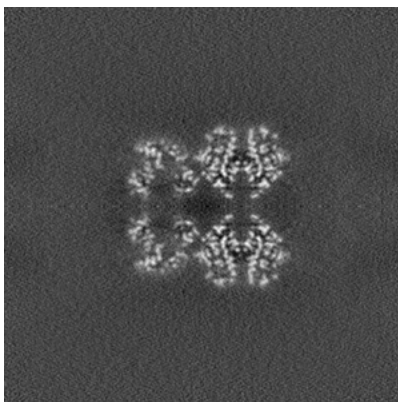


Z Index: 181

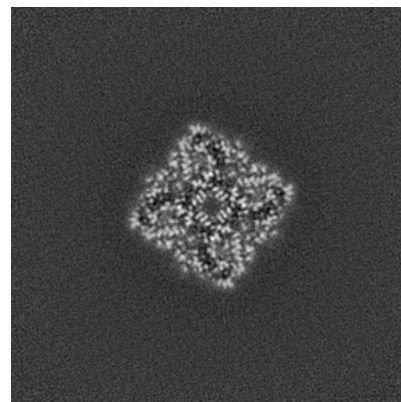
### 6.3.2 Raw map



X Index: 160



Y Index: 160



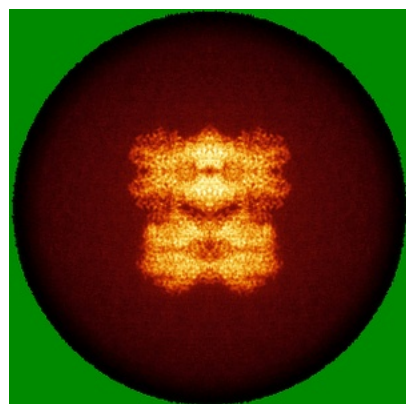
Z Index: 203

The images above show the largest variance slices of the map in three orthogonal directions.

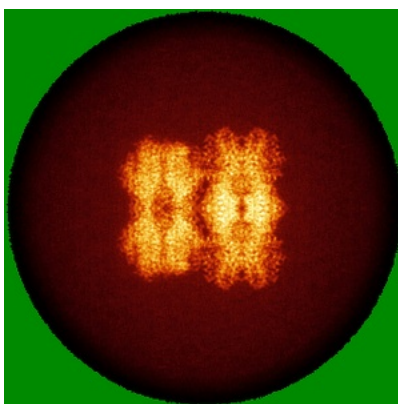


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

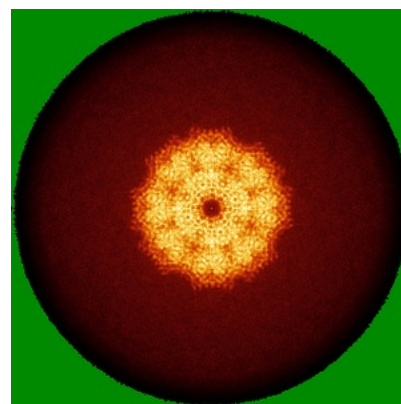
### 6.4.1 Primary map



X

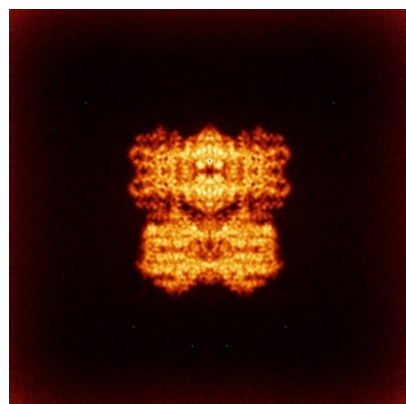


Y

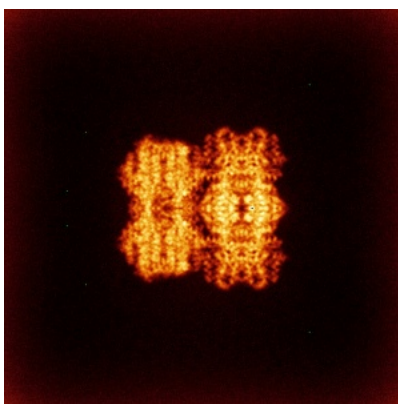


Z

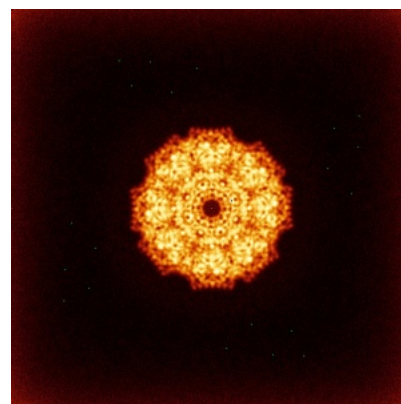
### 6.4.2 Raw map



X



Y

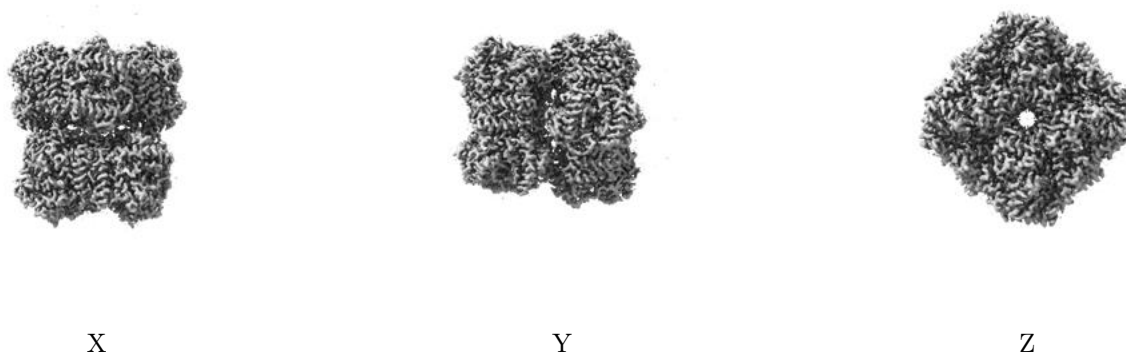


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

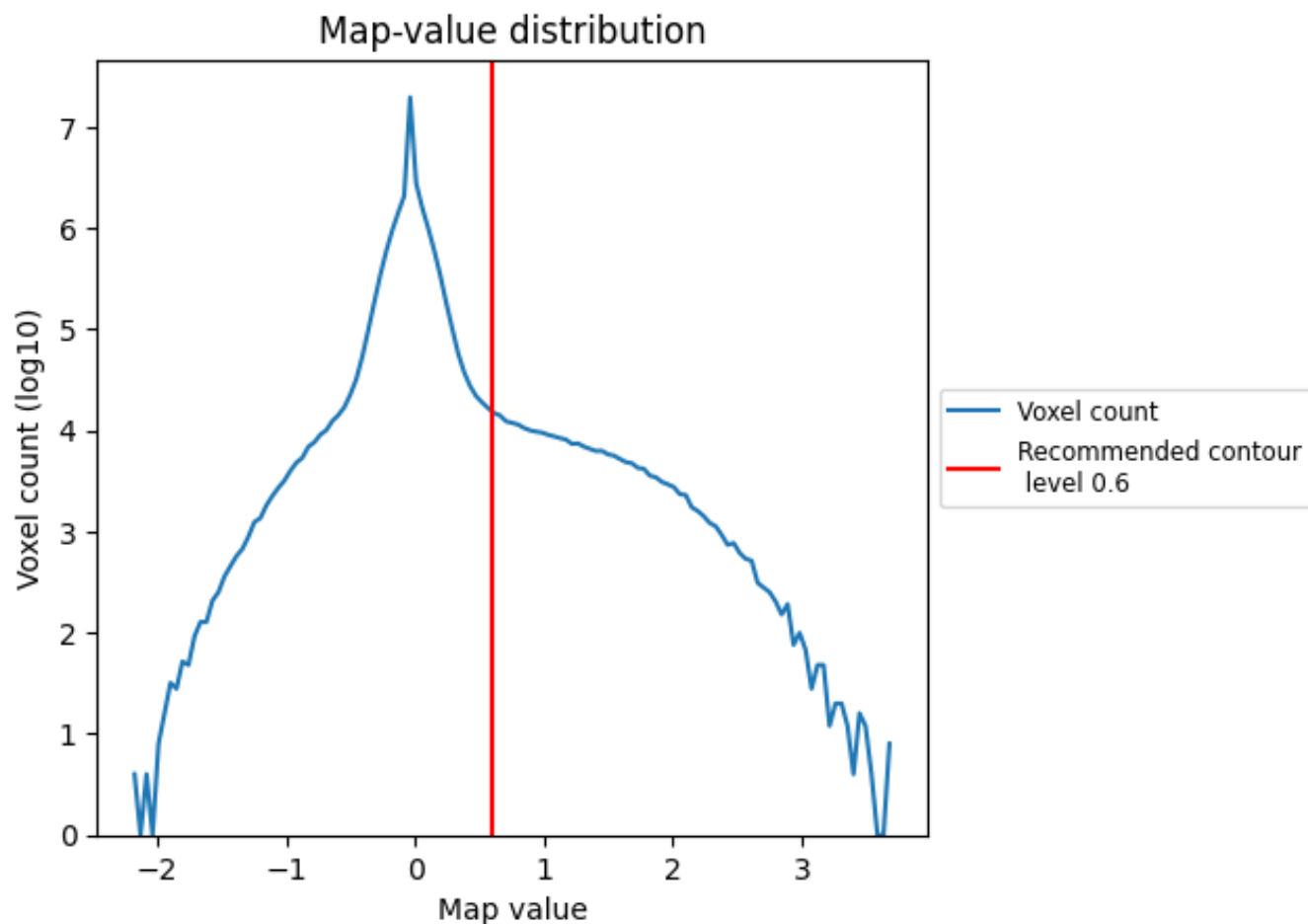
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

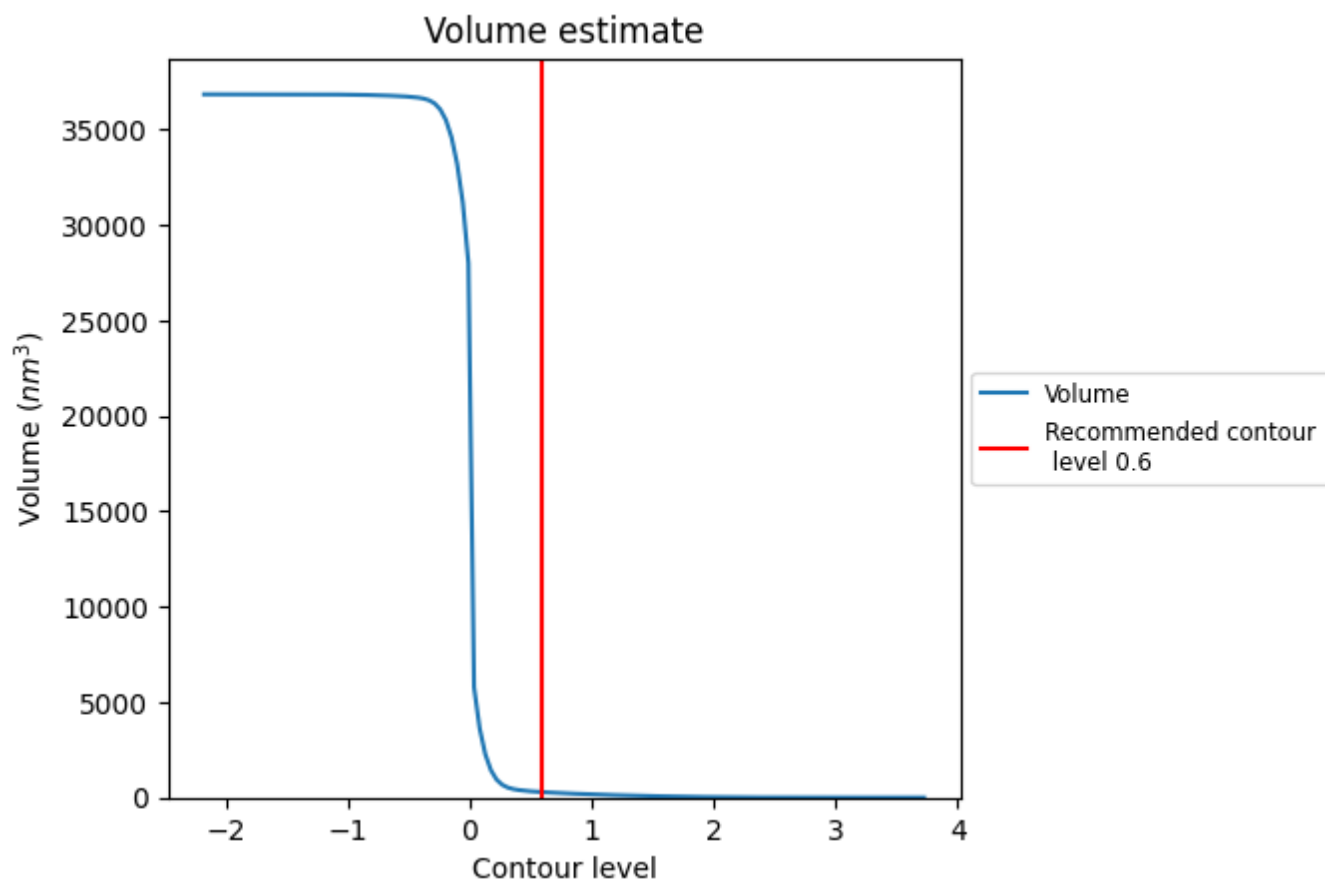
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

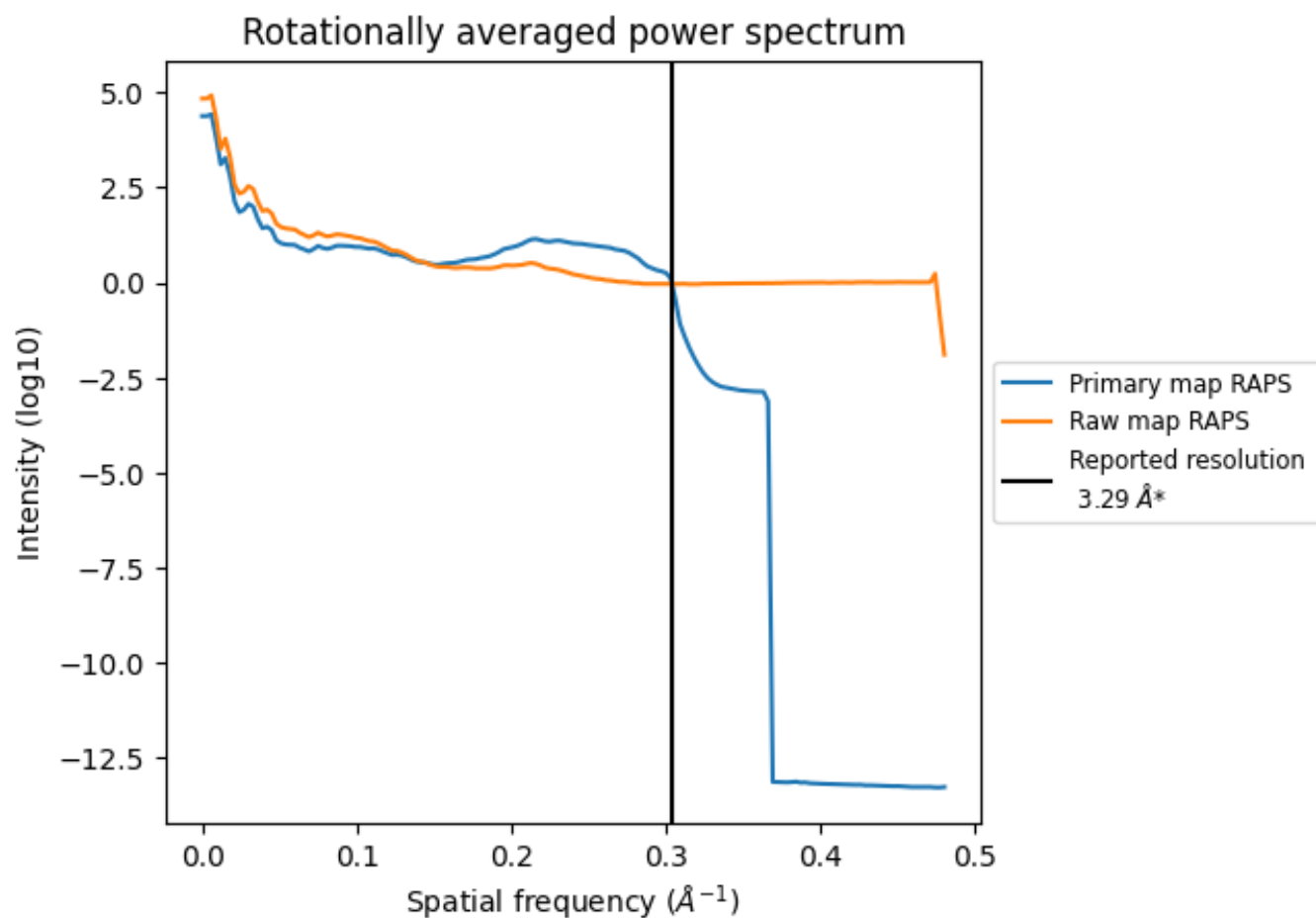
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 284 nm<sup>3</sup>; this corresponds to an approximate mass of 257 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

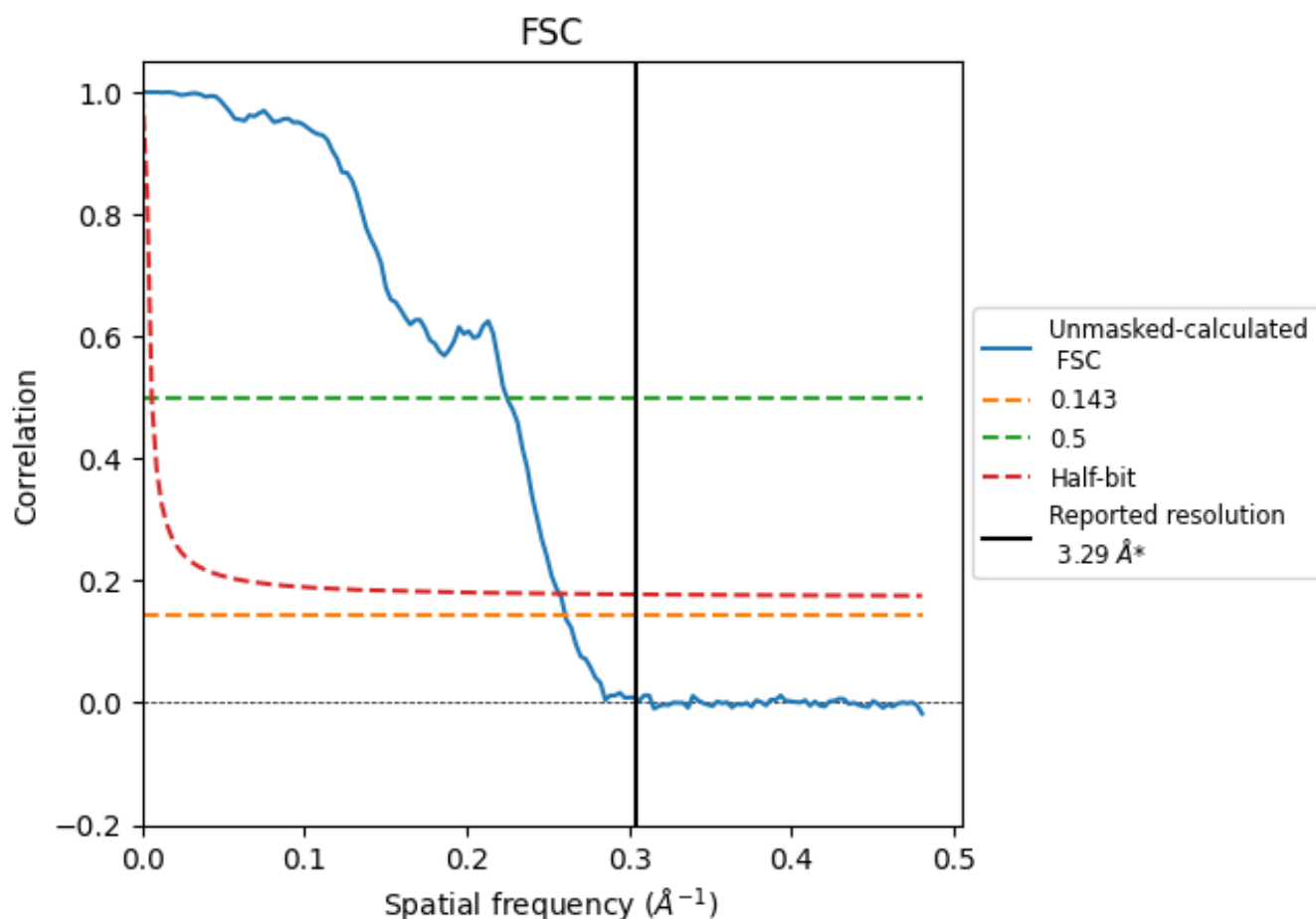


\*Reported resolution corresponds to spatial frequency of 0.304 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.304  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

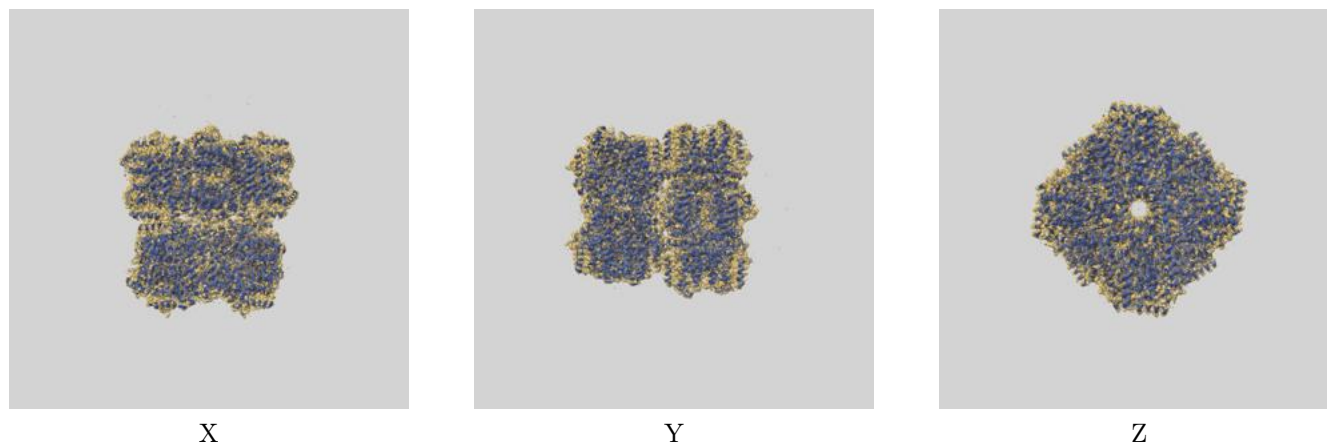
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.29                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.83                               | 4.45 | 3.89     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 3.29 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65396 and PDB model 9VWG. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

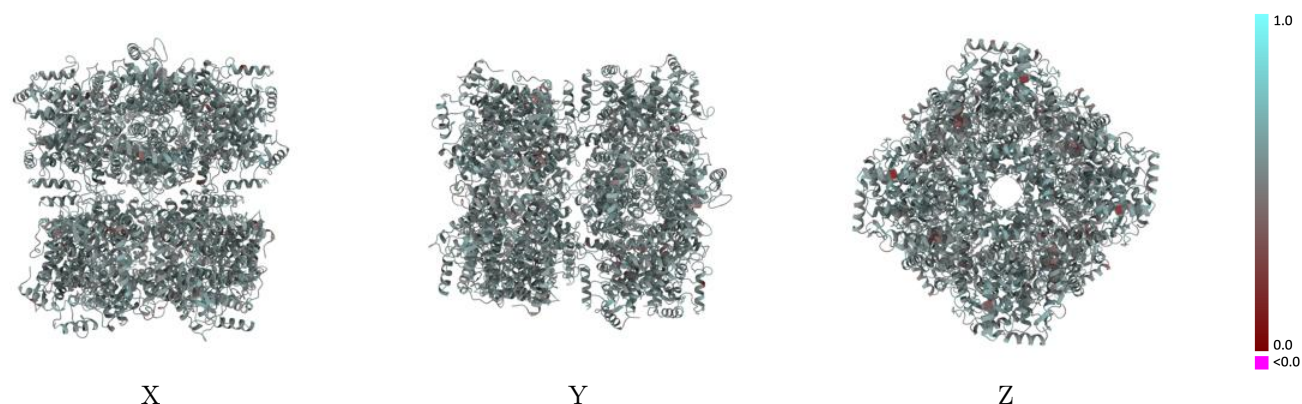
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

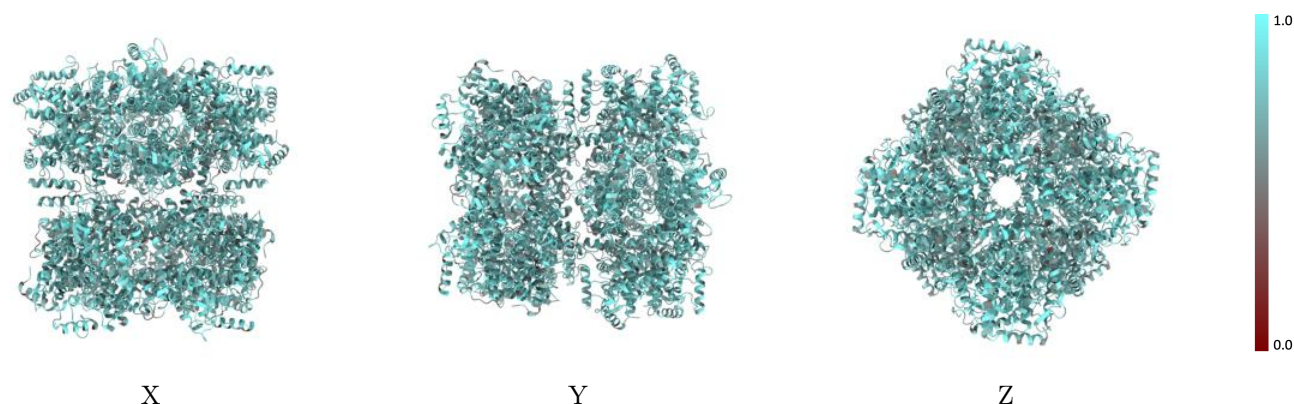


## 9.2 Q-score mapped to coordinate model [i](#)



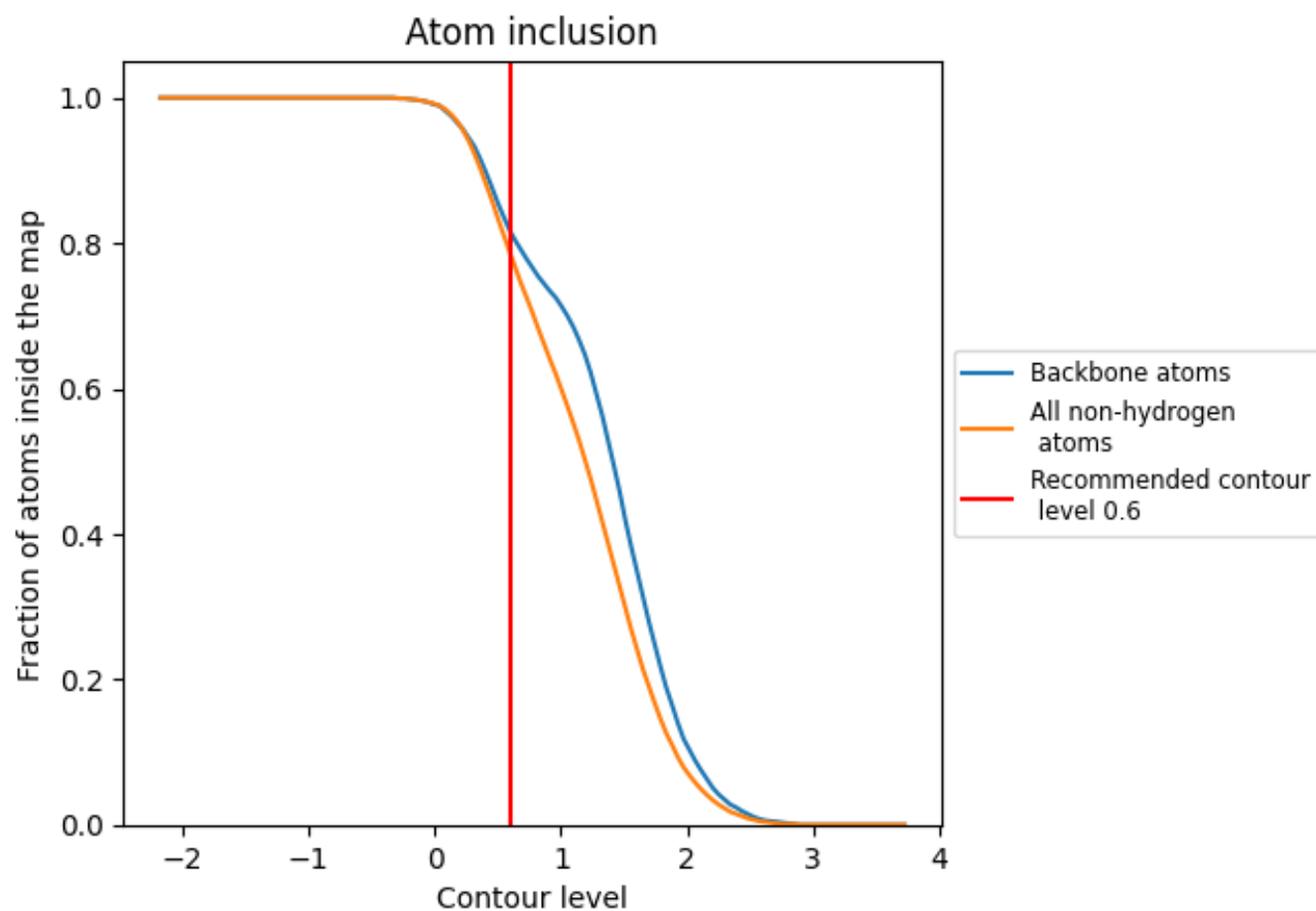
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.7850 | <div><div></div></div> 0.5430 |
| A     | <div><div></div></div> 0.7800 | <div><div></div></div> 0.5420 |
| B     | <div><div></div></div> 0.7810 | <div><div></div></div> 0.5430 |
| C     | <div><div></div></div> 0.7740 | <div><div></div></div> 0.5400 |
| D     | <div><div></div></div> 0.7760 | <div><div></div></div> 0.5410 |
| E     | <div><div></div></div> 0.7840 | <div><div></div></div> 0.5450 |
| F     | <div><div></div></div> 0.7810 | <div><div></div></div> 0.5440 |
| G     | <div><div></div></div> 0.7730 | <div><div></div></div> 0.5390 |
| H     | <div><div></div></div> 0.7810 | <div><div></div></div> 0.5450 |
| I     | <div><div></div></div> 0.7910 | <div><div></div></div> 0.5440 |
| J     | <div><div></div></div> 0.7910 | <div><div></div></div> 0.5440 |
| K     | <div><div></div></div> 0.7860 | <div><div></div></div> 0.5450 |
| L     | <div><div></div></div> 0.7930 | <div><div></div></div> 0.5460 |
| M     | <div><div></div></div> 0.7890 | <div><div></div></div> 0.5430 |
| N     | <div><div></div></div> 0.7890 | <div><div></div></div> 0.5420 |
| O     | <div><div></div></div> 0.7900 | <div><div></div></div> 0.5440 |
| P     | <div><div></div></div> 0.7930 | <div><div></div></div> 0.5450 |

1.0

0.0

<0.0