



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:04 PM UTC

PDB ID : 8AKS / pdb\_00008aks  
EMDB ID : EMD-15491  
Title : 215 A SynPspA rod after incubation with ATP  
Authors : Junglas, B.; Hudina, E.; Schoennenbeck, P.; Ritter, I.; Santiago-Schuebel, B.;  
Huesgen, P.; Sachse, C.  
Deposited on : 2022-07-31  
Resolution : 3.90 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:

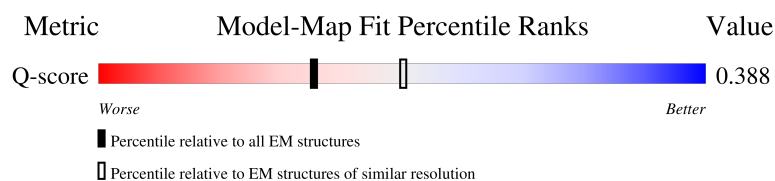
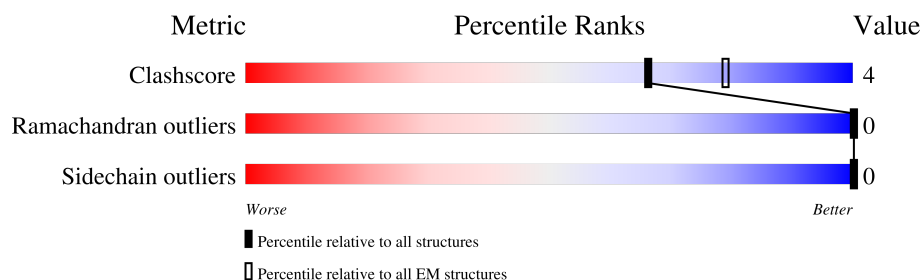
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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) : 2.49

# 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 3.90 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                       | 8855 ( 3.40 - 4.40 )                                     |

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   | 0     | 246    |                  |
| 1   | 1     | 246    |                  |
| 1   | 2     | 246    |                  |
| 1   | 3     | 246    |                  |

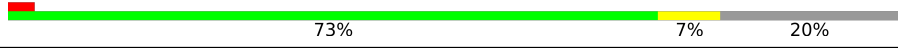
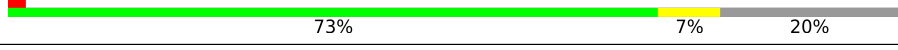
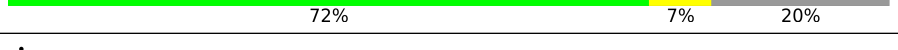
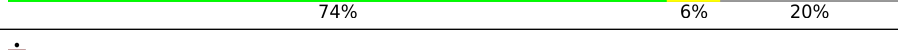
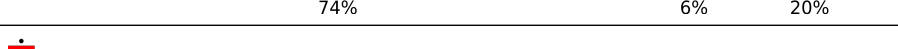
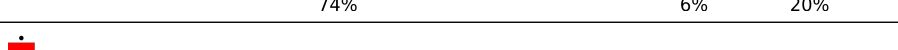
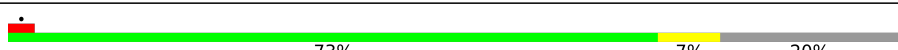
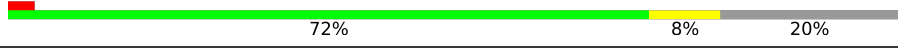
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 4     | 246    |                  |
| 1   | 5     | 246    |                  |
| 1   | 6     | 246    |                  |
| 1   | 7     | 246    |                  |
| 1   | A     | 246    |                  |
| 1   | B     | 246    |                  |
| 1   | C     | 246    |                  |
| 1   | D     | 246    |                  |
| 1   | E     | 246    |                  |
| 1   | F     | 246    |                  |
| 1   | G     | 246    |                  |
| 1   | H     | 246    |                  |
| 1   | I     | 246    |                  |
| 1   | J     | 246    |                  |
| 1   | K     | 246    |                  |
| 1   | L     | 246    |                  |
| 1   | M     | 246    |                  |
| 1   | N     | 246    |                  |
| 1   | O     | 246    |                  |
| 1   | P     | 246    |                  |
| 1   | Q     | 246    |                  |
| 1   | R     | 246    |                  |
| 1   | S     | 246    |                  |
| 1   | T     | 246    |                  |
| 1   | U     | 246    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | V     | 246    |    |
| 1   | W     | 246    |    |
| 1   | X     | 246    |    |
| 1   | Y     | 246    |    |
| 1   | Z     | 246    |    |
| 1   | a     | 246    |    |
| 1   | b     | 246    |    |
| 1   | c     | 246    |    |
| 1   | d     | 246    |    |
| 1   | e     | 246    |    |
| 1   | f     | 246    |    |
| 1   | g     | 246    |  |
| 1   | h     | 246    |  |
| 1   | i     | 246    |  |
| 1   | j     | 246    |  |
| 1   | k     | 246    |  |
| 1   | l     | 246    |  |
| 1   | m     | 246    |  |
| 1   | n     | 246    |  |
| 1   | o     | 246    |  |
| 1   | p     | 246    |  |
| 1   | q     | 246    |  |
| 1   | r     | 246    |  |
| 1   | s     | 246    |  |
| 1   | t     | 246    |  |

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| Mol | Chain | Length | Quality of chain                                                             |
|-----|-------|--------|------------------------------------------------------------------------------|
| 1   | u     | 246    | <div><div><div>9%</div><div>74%</div><div>6%</div><div>20%</div></div></div> |
| 1   | v     | 246    | <div><div><div></div><div>74%</div><div>6%</div><div>20%</div></div></div>   |
| 1   | w     | 246    | <div><div><div></div><div>73%</div><div>7%</div><div>20%</div></div></div>   |
| 1   | x     | 246    | <div><div><div></div><div>74%</div><div>6%</div><div>20%</div></div></div>   |
| 1   | y     | 246    | <div><div><div></div><div>74%</div><div>5%</div><div>20%</div></div></div>   |
| 1   | z     | 246    | <div><div><div></div><div>73%</div><div>7%</div><div>20%</div></div></div>   |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 107640 atoms, of which 11400 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 Chloroplast membrane-associated 30 kD protein.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 1   | 0     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | 1     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | 2     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | 3     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | 4     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | 5     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | 6     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | 7     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | A     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | B     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | C     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | D     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | E     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | F     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | G     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | H     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | I     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 1   | J     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | K     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | L     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | M     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | N     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | O     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | P     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | Q     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | R     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | S     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | T     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | U     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | V     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | W     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | X     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | Y     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | Z     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | a     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | b     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | c     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | d     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 1   | e     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | f     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | g     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | h     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | i     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | j     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | k     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | l     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | m     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | n     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | o     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | p     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | q     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | r     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | s     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | t     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | u     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | v     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | w     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | x     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |
| 1   | y     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 1   | z     | 196      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1767  | 978 | 190 | 289 | 308 | 2 |         |       |

There are 1380 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 0     | -22     | MET      | -      | initiating methionine | UNP P74717 |
| 0     | -21     | GLY      | -      | expression tag        | UNP P74717 |
| 0     | -20     | SER      | -      | expression tag        | UNP P74717 |
| 0     | -19     | SER      | -      | expression tag        | UNP P74717 |
| 0     | -18     | HIS      | -      | expression tag        | UNP P74717 |
| 0     | -17     | HIS      | -      | expression tag        | UNP P74717 |
| 0     | -16     | HIS      | -      | expression tag        | UNP P74717 |
| 0     | -15     | HIS      | -      | expression tag        | UNP P74717 |
| 0     | -14     | HIS      | -      | expression tag        | UNP P74717 |
| 0     | -13     | HIS      | -      | expression tag        | UNP P74717 |
| 0     | -12     | SER      | -      | expression tag        | UNP P74717 |
| 0     | -11     | SER      | -      | expression tag        | UNP P74717 |
| 0     | -10     | SER      | -      | expression tag        | UNP P74717 |
| 0     | -9      | ALA      | -      | expression tag        | UNP P74717 |
| 0     | -8      | ALA      | -      | expression tag        | UNP P74717 |
| 0     | -7      | LEU      | -      | expression tag        | UNP P74717 |
| 0     | -6      | GLU      | -      | expression tag        | UNP P74717 |
| 0     | -5      | VAL      | -      | expression tag        | UNP P74717 |
| 0     | -4      | LEU      | -      | expression tag        | UNP P74717 |
| 0     | -3      | PHE      | -      | expression tag        | UNP P74717 |
| 0     | -2      | GLN      | -      | expression tag        | UNP P74717 |
| 0     | -1      | GLY      | -      | expression tag        | UNP P74717 |
| 0     | 0       | PRO      | -      | expression tag        | UNP P74717 |
| 1     | -22     | MET      | -      | initiating methionine | UNP P74717 |
| 1     | -21     | GLY      | -      | expression tag        | UNP P74717 |
| 1     | -20     | SER      | -      | expression tag        | UNP P74717 |
| 1     | -19     | SER      | -      | expression tag        | UNP P74717 |
| 1     | -18     | HIS      | -      | expression tag        | UNP P74717 |
| 1     | -17     | HIS      | -      | expression tag        | UNP P74717 |
| 1     | -16     | HIS      | -      | expression tag        | UNP P74717 |
| 1     | -15     | HIS      | -      | expression tag        | UNP P74717 |
| 1     | -14     | HIS      | -      | expression tag        | UNP P74717 |
| 1     | -13     | HIS      | -      | expression tag        | UNP P74717 |
| 1     | -12     | SER      | -      | expression tag        | UNP P74717 |
| 1     | -11     | SER      | -      | expression tag        | UNP P74717 |
| 1     | -10     | SER      | -      | expression tag        | UNP P74717 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 1     | -9      | ALA      | -      | expression tag        | UNP P74717 |
| 1     | -8      | ALA      | -      | expression tag        | UNP P74717 |
| 1     | -7      | LEU      | -      | expression tag        | UNP P74717 |
| 1     | -6      | GLU      | -      | expression tag        | UNP P74717 |
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| 3     | -15     | HIS      | -      | expression tag        | UNP P74717 |
| 3     | -14     | HIS      | -      | expression tag        | UNP P74717 |

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*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| 5     | -19     | SER      | -      | expression tag        | UNP P74717 |
| 5     | -18     | HIS      | -      | expression tag        | UNP P74717 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| 6     | 0       | PRO      | -      | expression tag        | UNP P74717 |
| 7     | -22     | MET      | -      | initiating methionine | UNP P74717 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
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| A     | -4      | LEU      | -      | expression tag        | UNP P74717 |
| A     | -3      | PHE      | -      | expression tag        | UNP P74717 |

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*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
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| B     | -22     | MET      | -      | initiating methionine | UNP P74717 |
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| C     | -8      | ALA      | -      | expression tag        | UNP P74717 |
| C     | -7      | LEU      | -      | expression tag        | UNP P74717 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| C     | -3      | PHE      | -      | expression tag        | UNP P74717 |
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| C     | -1      | GLY      | -      | expression tag        | UNP P74717 |
| C     | 0       | PRO      | -      | expression tag        | UNP P74717 |
| D     | -22     | MET      | -      | initiating methionine | UNP P74717 |
| D     | -21     | GLY      | -      | expression tag        | UNP P74717 |
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| D     | -19     | SER      | -      | expression tag        | UNP P74717 |
| D     | -18     | HIS      | -      | expression tag        | UNP P74717 |
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| D     | -1      | GLY      | -      | expression tag        | UNP P74717 |
| D     | 0       | PRO      | -      | expression tag        | UNP P74717 |
| E     | -22     | MET      | -      | initiating methionine | UNP P74717 |
| E     | -21     | GLY      | -      | expression tag        | UNP P74717 |
| E     | -20     | SER      | -      | expression tag        | UNP P74717 |
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*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| E     | -1      | GLY      | -      | expression tag        | UNP P74717 |
| E     | 0       | PRO      | -      | expression tag        | UNP P74717 |
| F     | -22     | MET      | -      | initiating methionine | UNP P74717 |
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| F     | -1      | GLY      | -      | expression tag        | UNP P74717 |
| F     | 0       | PRO      | -      | expression tag        | UNP P74717 |
| G     | -22     | MET      | -      | initiating methionine | UNP P74717 |
| G     | -21     | GLY      | -      | expression tag        | UNP P74717 |
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| G     | -18     | HIS      | -      | expression tag        | UNP P74717 |
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| G     | -16     | HIS      | -      | expression tag        | UNP P74717 |
| G     | -15     | HIS      | -      | expression tag        | UNP P74717 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| G     | -14     | HIS      | -      | expression tag        | UNP P74717 |
| G     | -13     | HIS      | -      | expression tag        | UNP P74717 |
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| G     | -2      | GLN      | -      | expression tag        | UNP P74717 |
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| H     | 0       | PRO      | -      | expression tag        | UNP P74717 |
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| I     | -21     | GLY      | -      | expression tag        | UNP P74717 |
| I     | -20     | SER      | -      | expression tag        | UNP P74717 |
| I     | -19     | SER      | -      | expression tag        | UNP P74717 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| I     | -18     | HIS      | -      | expression tag        | UNP P74717 |
| I     | -17     | HIS      | -      | expression tag        | UNP P74717 |
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| I     | -13     | HIS      | -      | expression tag        | UNP P74717 |
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| I     | -11     | SER      | -      | expression tag        | UNP P74717 |
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| I     | -8      | ALA      | -      | expression tag        | UNP P74717 |
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| I     | -6      | GLU      | -      | expression tag        | UNP P74717 |
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| J     | -1      | GLY      | -      | expression tag        | UNP P74717 |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| N     | -1      | GLY      | -      | expression tag        | UNP P74717 |
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*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Q     | -21     | GLY      | -      | expression tag        | UNP P74717 |
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| R     | -22     | MET      | -      | initiating methionine | UNP P74717 |
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*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| R     | -1      | GLY      | -      | expression tag        | UNP P74717 |
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| S     | -21     | GLY      | -      | expression tag        | UNP P74717 |
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| S     | -18     | HIS      | -      | expression tag        | UNP P74717 |
| S     | -17     | HIS      | -      | expression tag        | UNP P74717 |
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| T     | -21     | GLY      | -      | expression tag        | UNP P74717 |
| T     | -20     | SER      | -      | expression tag        | UNP P74717 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| e     | -22     | MET      | -      | initiating methionine | UNP P74717 |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| r     | -17     | HIS      | -      | expression tag        | UNP P74717 |
| r     | -16     | HIS      | -      | expression tag        | UNP P74717 |
| r     | -15     | HIS      | -      | expression tag        | UNP P74717 |
| r     | -14     | HIS      | -      | expression tag        | UNP P74717 |
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| r     | -12     | SER      | -      | expression tag        | UNP P74717 |
| r     | -11     | SER      | -      | expression tag        | UNP P74717 |
| r     | -10     | SER      | -      | expression tag        | UNP P74717 |
| r     | -9      | ALA      | -      | expression tag        | UNP P74717 |
| r     | -8      | ALA      | -      | expression tag        | UNP P74717 |
| r     | -7      | LEU      | -      | expression tag        | UNP P74717 |
| r     | -6      | GLU      | -      | expression tag        | UNP P74717 |
| r     | -5      | VAL      | -      | expression tag        | UNP P74717 |
| r     | -4      | LEU      | -      | expression tag        | UNP P74717 |
| r     | -3      | PHE      | -      | expression tag        | UNP P74717 |
| r     | -2      | GLN      | -      | expression tag        | UNP P74717 |
| r     | -1      | GLY      | -      | expression tag        | UNP P74717 |
| r     | 0       | PRO      | -      | expression tag        | UNP P74717 |
| s     | -22     | MET      | -      | initiating methionine | UNP P74717 |
| s     | -21     | GLY      | -      | expression tag        | UNP P74717 |
| s     | -20     | SER      | -      | expression tag        | UNP P74717 |
| s     | -19     | SER      | -      | expression tag        | UNP P74717 |
| s     | -18     | HIS      | -      | expression tag        | UNP P74717 |
| s     | -17     | HIS      | -      | expression tag        | UNP P74717 |
| s     | -16     | HIS      | -      | expression tag        | UNP P74717 |
| s     | -15     | HIS      | -      | expression tag        | UNP P74717 |
| s     | -14     | HIS      | -      | expression tag        | UNP P74717 |
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| s     | -11     | SER      | -      | expression tag        | UNP P74717 |
| s     | -10     | SER      | -      | expression tag        | UNP P74717 |
| s     | -9      | ALA      | -      | expression tag        | UNP P74717 |
| s     | -8      | ALA      | -      | expression tag        | UNP P74717 |
| s     | -7      | LEU      | -      | expression tag        | UNP P74717 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| s     | -6      | GLU      | -      | expression tag        | UNP P74717 |
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| s     | -3      | PHE      | -      | expression tag        | UNP P74717 |
| s     | -2      | GLN      | -      | expression tag        | UNP P74717 |
| s     | -1      | GLY      | -      | expression tag        | UNP P74717 |
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| t     | -21     | GLY      | -      | expression tag        | UNP P74717 |
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| t     | -4      | LEU      | -      | expression tag        | UNP P74717 |
| t     | -3      | PHE      | -      | expression tag        | UNP P74717 |
| t     | -2      | GLN      | -      | expression tag        | UNP P74717 |
| t     | -1      | GLY      | -      | expression tag        | UNP P74717 |
| t     | 0       | PRO      | -      | expression tag        | UNP P74717 |
| u     | -22     | MET      | -      | initiating methionine | UNP P74717 |
| u     | -21     | GLY      | -      | expression tag        | UNP P74717 |
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| u     | -13     | HIS      | -      | expression tag        | UNP P74717 |
| u     | -12     | SER      | -      | expression tag        | UNP P74717 |
| u     | -11     | SER      | -      | expression tag        | UNP P74717 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
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| u     | -7      | LEU      | -      | expression tag        | UNP P74717 |
| u     | -6      | GLU      | -      | expression tag        | UNP P74717 |
| u     | -5      | VAL      | -      | expression tag        | UNP P74717 |
| u     | -4      | LEU      | -      | expression tag        | UNP P74717 |
| u     | -3      | PHE      | -      | expression tag        | UNP P74717 |
| u     | -2      | GLN      | -      | expression tag        | UNP P74717 |
| u     | -1      | GLY      | -      | expression tag        | UNP P74717 |
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| v     | -17     | HIS      | -      | expression tag        | UNP P74717 |
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| v     | -1      | GLY      | -      | expression tag        | UNP P74717 |
| v     | 0       | PRO      | -      | expression tag        | UNP P74717 |
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| w     | -16     | HIS      | -      | expression tag        | UNP P74717 |
| w     | -15     | HIS      | -      | expression tag        | UNP P74717 |

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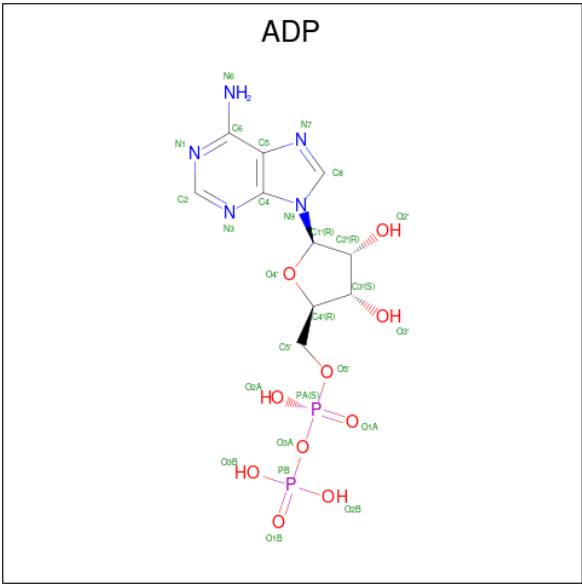
| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| w     | -14     | HIS      | -      | expression tag        | UNP P74717 |
| w     | -13     | HIS      | -      | expression tag        | UNP P74717 |
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| w     | -11     | SER      | -      | expression tag        | UNP P74717 |
| w     | -10     | SER      | -      | expression tag        | UNP P74717 |
| w     | -9      | ALA      | -      | expression tag        | UNP P74717 |
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| w     | -7      | LEU      | -      | expression tag        | UNP P74717 |
| w     | -6      | GLU      | -      | expression tag        | UNP P74717 |
| w     | -5      | VAL      | -      | expression tag        | UNP P74717 |
| w     | -4      | LEU      | -      | expression tag        | UNP P74717 |
| w     | -3      | PHE      | -      | expression tag        | UNP P74717 |
| w     | -2      | GLN      | -      | expression tag        | UNP P74717 |
| w     | -1      | GLY      | -      | expression tag        | UNP P74717 |
| w     | 0       | PRO      | -      | expression tag        | UNP P74717 |
| x     | -22     | MET      | -      | initiating methionine | UNP P74717 |
| x     | -21     | GLY      | -      | expression tag        | UNP P74717 |
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| x     | -19     | SER      | -      | expression tag        | UNP P74717 |
| x     | -18     | HIS      | -      | expression tag        | UNP P74717 |
| x     | -17     | HIS      | -      | expression tag        | UNP P74717 |
| x     | -16     | HIS      | -      | expression tag        | UNP P74717 |
| x     | -15     | HIS      | -      | expression tag        | UNP P74717 |
| x     | -14     | HIS      | -      | expression tag        | UNP P74717 |
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| x     | -12     | SER      | -      | expression tag        | UNP P74717 |
| x     | -11     | SER      | -      | expression tag        | UNP P74717 |
| x     | -10     | SER      | -      | expression tag        | UNP P74717 |
| x     | -9      | ALA      | -      | expression tag        | UNP P74717 |
| x     | -8      | ALA      | -      | expression tag        | UNP P74717 |
| x     | -7      | LEU      | -      | expression tag        | UNP P74717 |
| x     | -6      | GLU      | -      | expression tag        | UNP P74717 |
| x     | -5      | VAL      | -      | expression tag        | UNP P74717 |
| x     | -4      | LEU      | -      | expression tag        | UNP P74717 |
| x     | -3      | PHE      | -      | expression tag        | UNP P74717 |
| x     | -2      | GLN      | -      | expression tag        | UNP P74717 |
| x     | -1      | GLY      | -      | expression tag        | UNP P74717 |
| x     | 0       | PRO      | -      | expression tag        | UNP P74717 |
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| y     | -21     | GLY      | -      | expression tag        | UNP P74717 |
| y     | -20     | SER      | -      | expression tag        | UNP P74717 |
| y     | -19     | SER      | -      | expression tag        | UNP P74717 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| y     | -18     | HIS      | -      | expression tag        | UNP P74717 |
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| y     | -15     | HIS      | -      | expression tag        | UNP P74717 |
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| y     | -9      | ALA      | -      | expression tag        | UNP P74717 |
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| y     | -7      | LEU      | -      | expression tag        | UNP P74717 |
| y     | -6      | GLU      | -      | expression tag        | UNP P74717 |
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| y     | -4      | LEU      | -      | expression tag        | UNP P74717 |
| y     | -3      | PHE      | -      | expression tag        | UNP P74717 |
| y     | -2      | GLN      | -      | expression tag        | UNP P74717 |
| y     | -1      | GLY      | -      | expression tag        | UNP P74717 |
| y     | 0       | PRO      | -      | expression tag        | UNP P74717 |
| z     | -22     | MET      | -      | initiating methionine | UNP P74717 |
| z     | -21     | GLY      | -      | expression tag        | UNP P74717 |
| z     | -20     | SER      | -      | expression tag        | UNP P74717 |
| z     | -19     | SER      | -      | expression tag        | UNP P74717 |
| z     | -18     | HIS      | -      | expression tag        | UNP P74717 |
| z     | -17     | HIS      | -      | expression tag        | UNP P74717 |
| z     | -16     | HIS      | -      | expression tag        | UNP P74717 |
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| z     | -11     | SER      | -      | expression tag        | UNP P74717 |
| z     | -10     | SER      | -      | expression tag        | UNP P74717 |
| z     | -9      | ALA      | -      | expression tag        | UNP P74717 |
| z     | -8      | ALA      | -      | expression tag        | UNP P74717 |
| z     | -7      | LEU      | -      | expression tag        | UNP P74717 |
| z     | -6      | GLU      | -      | expression tag        | UNP P74717 |
| z     | -5      | VAL      | -      | expression tag        | UNP P74717 |
| z     | -4      | LEU      | -      | expression tag        | UNP P74717 |
| z     | -3      | PHE      | -      | expression tag        | UNP P74717 |
| z     | -2      | GLN      | -      | expression tag        | UNP P74717 |
| z     | -1      | GLY      | -      | expression tag        | UNP P74717 |
| z     | 0       | PRO      | -      | expression tag        | UNP P74717 |

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 2   | 0     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | 1     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | 2     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | 3     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | 4     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | 5     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | 6     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | 7     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | B     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | C     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | D     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 2   | E     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | F     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | G     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | H     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | I     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | J     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | K     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | L     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | M     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | N     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | O     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | P     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | Q     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | R     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | S     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | T     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | U     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | V     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | W     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | X     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | Y     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 2   | Z     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | a     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | b     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | c     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | d     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | e     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | f     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | g     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | h     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | i     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | j     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | k     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | l     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | m     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | n     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | o     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | p     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | q     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | r     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | s     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 2   | t     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |

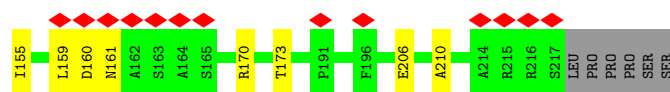
*Continued on next page...*

*Continued from previous page...*

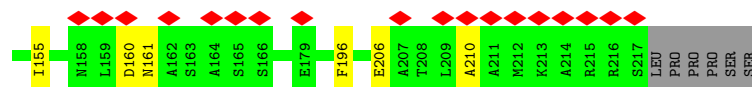
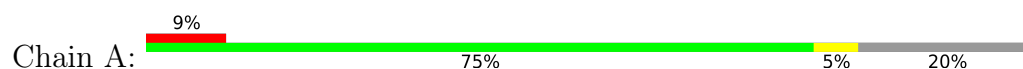
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|-----|-------|----------|-------|----|---|----|---|---------|
| 2   | u     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | v     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | w     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | x     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | y     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 2   | z     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |



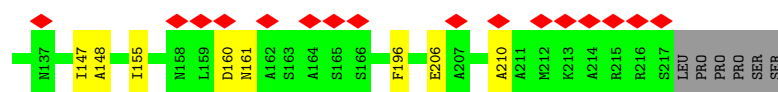
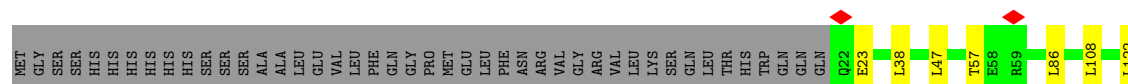
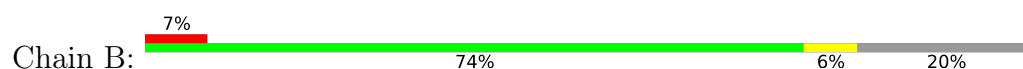




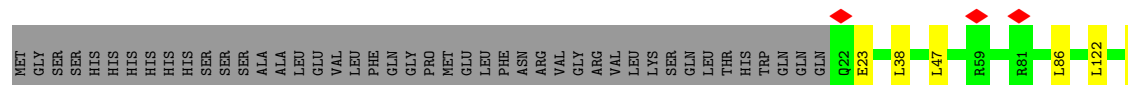
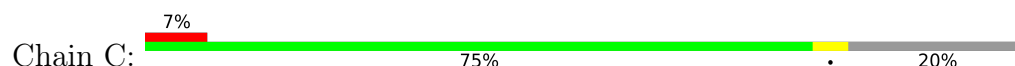
- Molecule 1: Chloroplast membrane-associated 30 kD protein



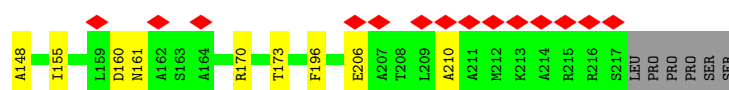
- Molecule 1: Chloroplast membrane-associated 30 kD protein



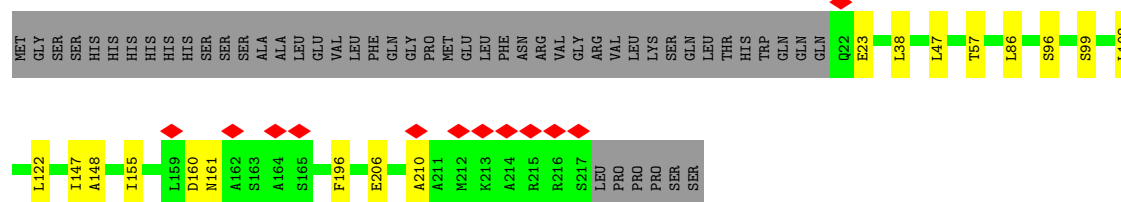
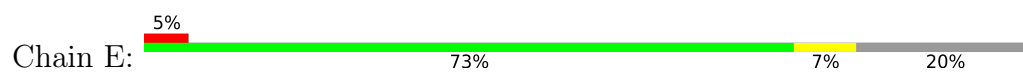
- Molecule 1: Chloroplast membrane-associated 30 kD protein



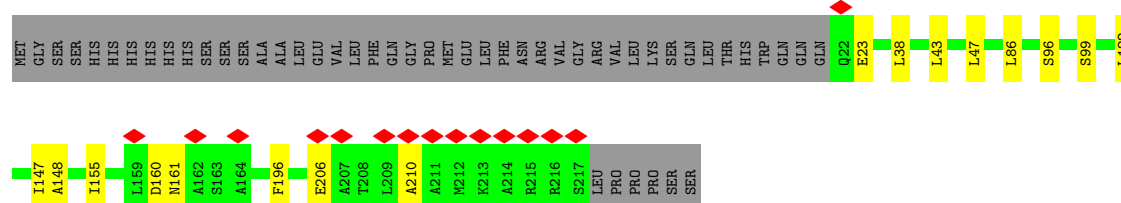
- Molecule 1: Chloroplast membrane-associated 30 kD protein



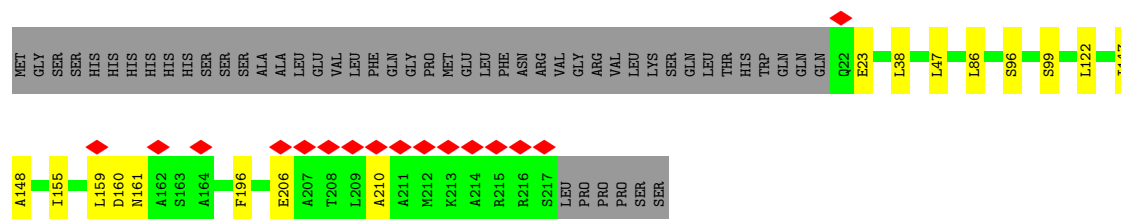
- Molecule 1: Chloroplast membrane-associated 30 kD protein



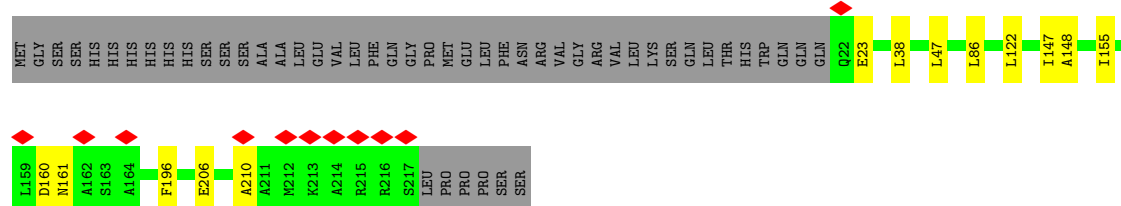
- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein

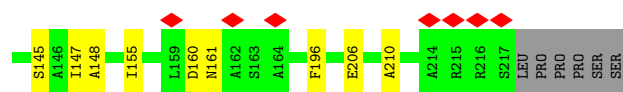


- Molecule 1: Chloroplast membrane-associated 30 kD protein



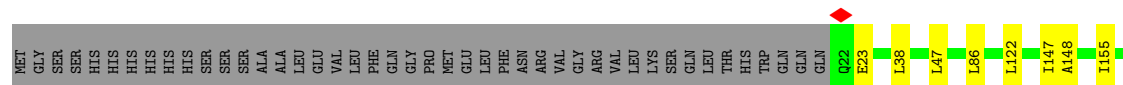
- Molecule 1: Chloroplast membrane-associated 30 kD protein





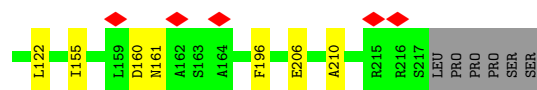
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain J: 74% 6% 20%



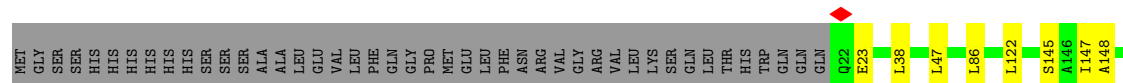
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain K: 74% 6% 20%



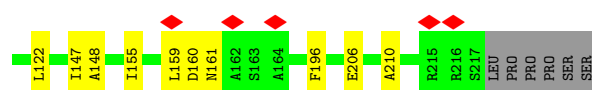
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain L: 74% 6% 20%

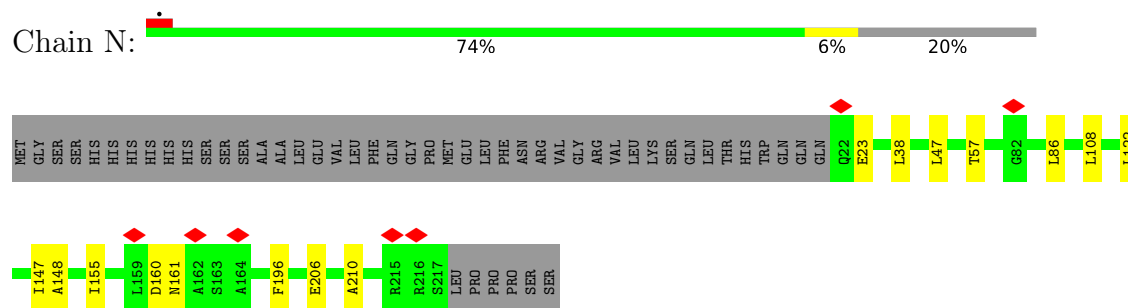


- Molecule 1: Chloroplast membrane-associated 30 kD protein

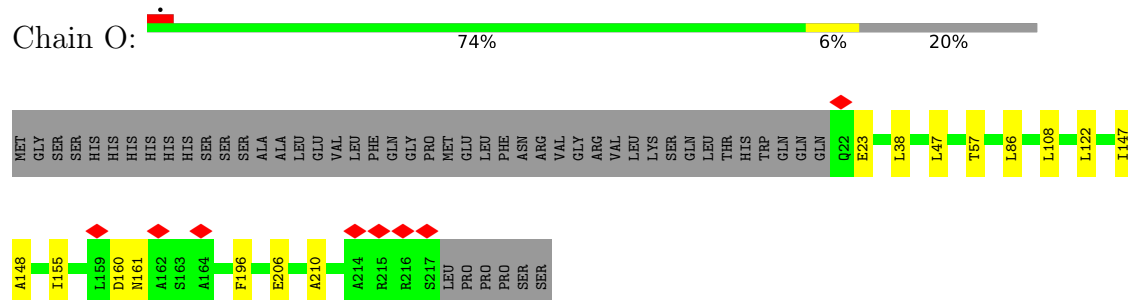
Chain M: 72% 7% 20%



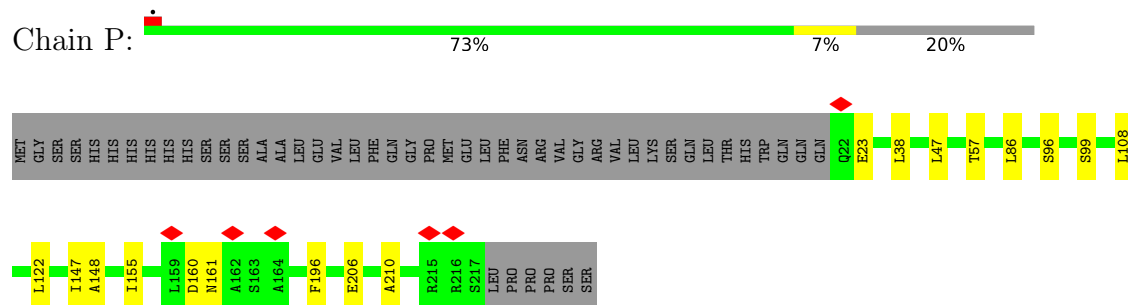
- Molecule 1: Chloroplast membrane-associated 30 kD protein



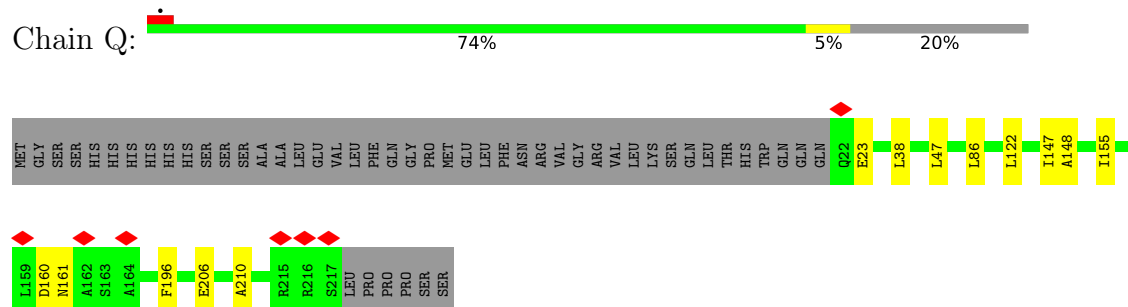
- Molecule 1: Chloroplast membrane-associated 30 kD protein



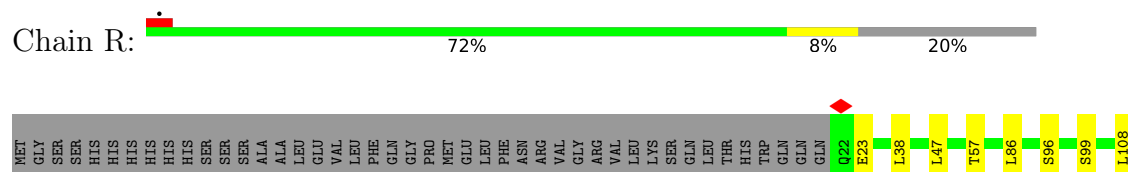
- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein



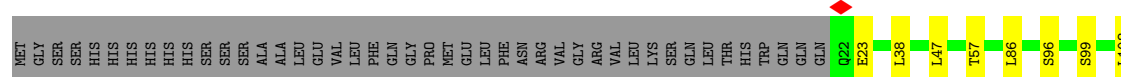
- Molecule 1: Chloroplast membrane-associated 30 kD protein





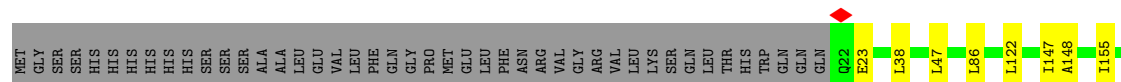
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain S: 73% 7% 20%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain T: 74% 5% 20%



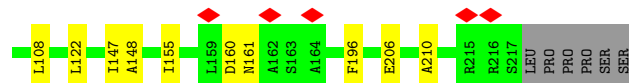
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain U: 74% 6% 20%



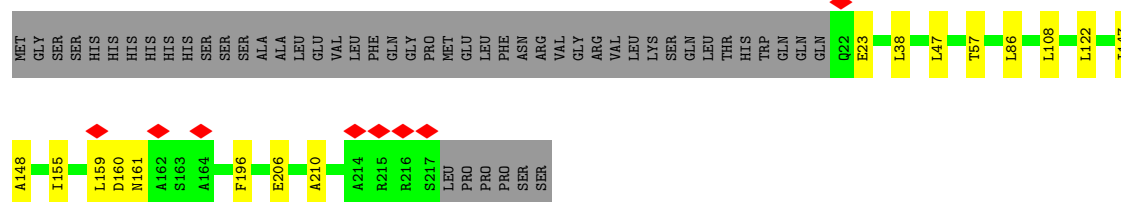
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain V: 73% 7% 20%



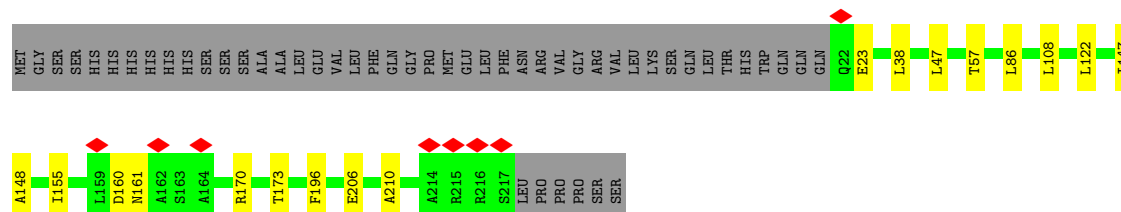
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain W: 



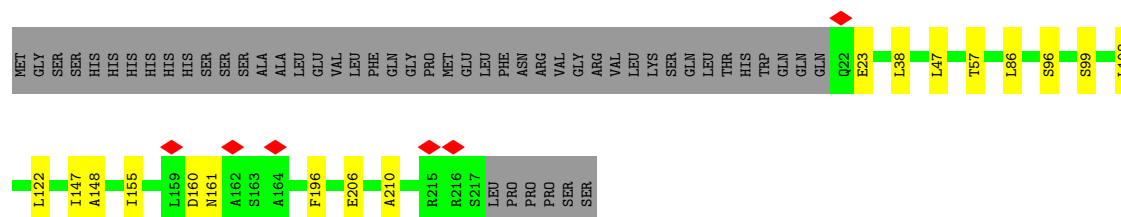
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain X: 



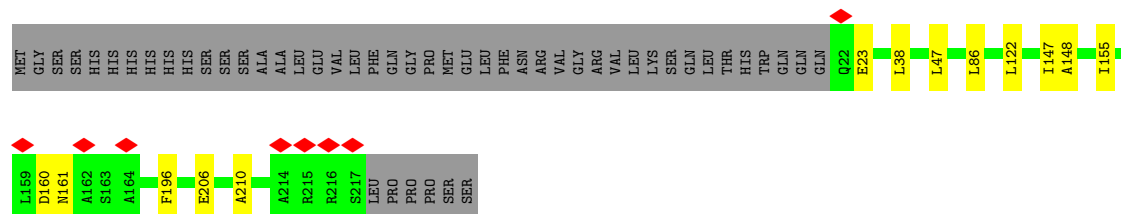
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain Y: 



- Molecule 1: Chloroplast membrane-associated 30 kD protein

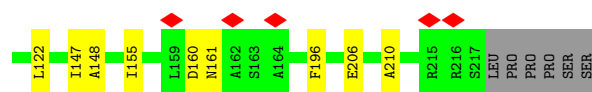
Chain Z: 



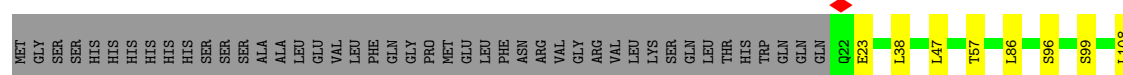
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain a: 

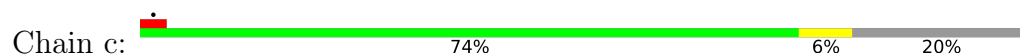




- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein

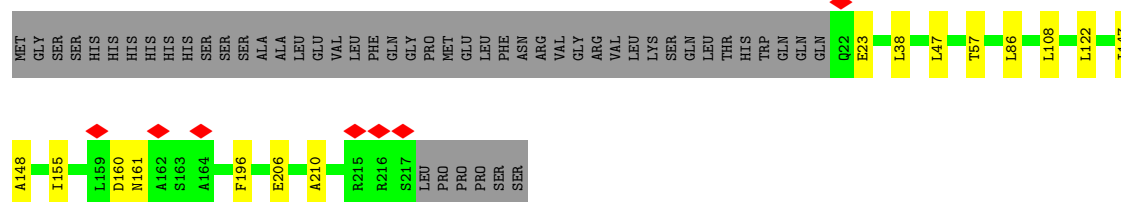


- Molecule 1: Chloroplast membrane-associated 30 kD protein



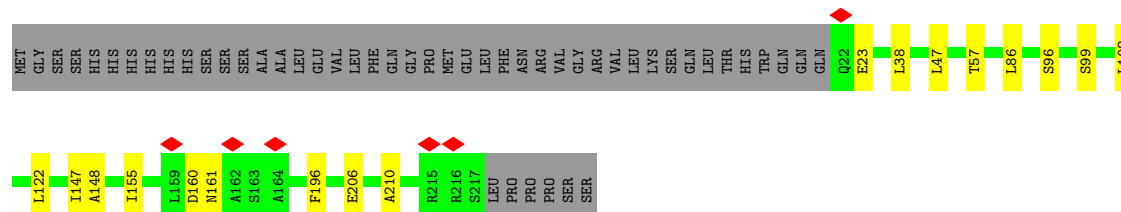
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain f:  74% 6% 20%



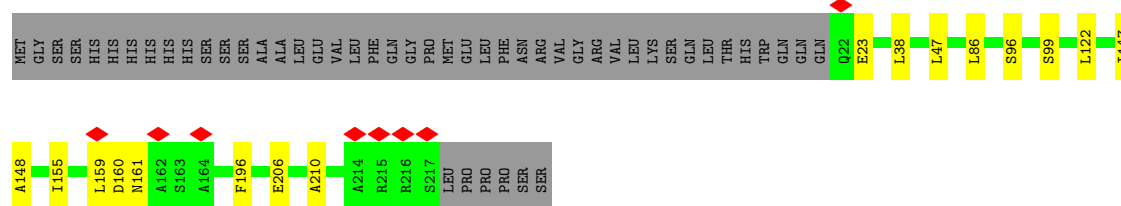
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain g:  73% 7% 20%



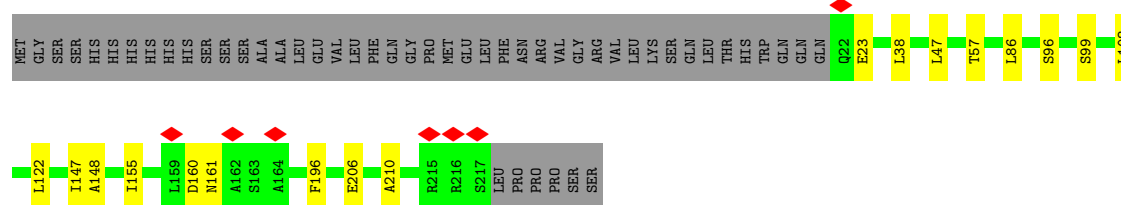
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain h:  73% 7% 20%



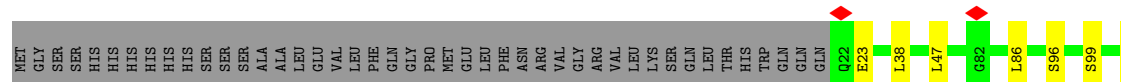
- Molecule 1: Chloroplast membrane-associated 30 kD protein

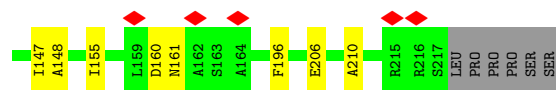
Chain i:  73% 7% 20%



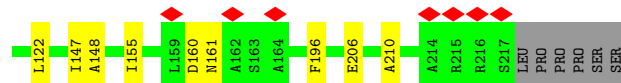
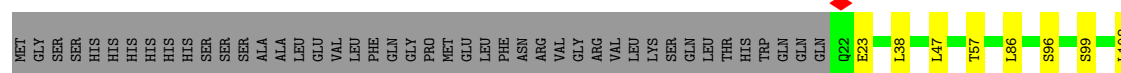
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain j:  74% 6% 20%

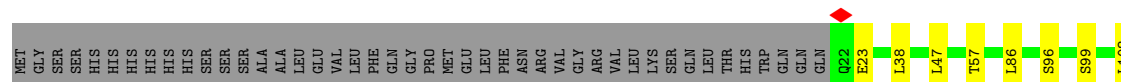




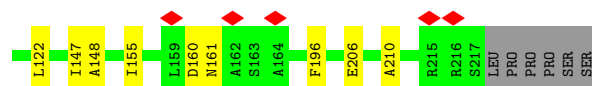
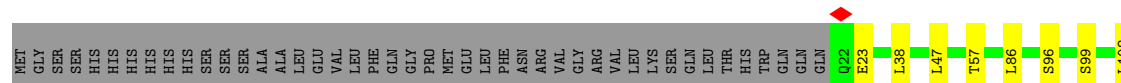
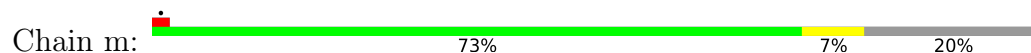
- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein



- Molecule 1: Chloroplast membrane-associated 30 kD protein

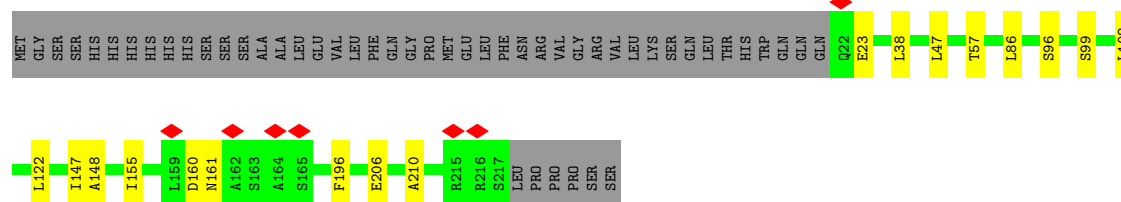


- Molecule 1: Chloroplast membrane-associated 30 kD protein



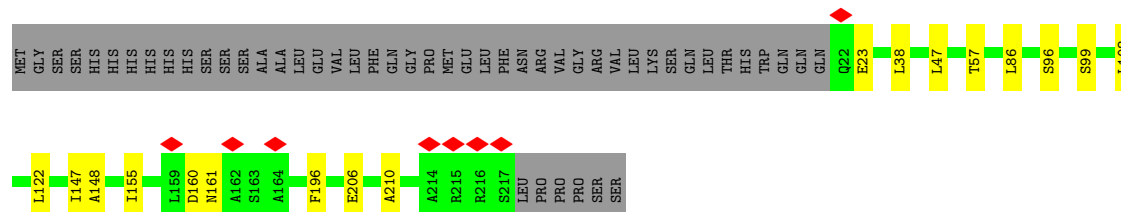
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain o:  73% 7% 20%



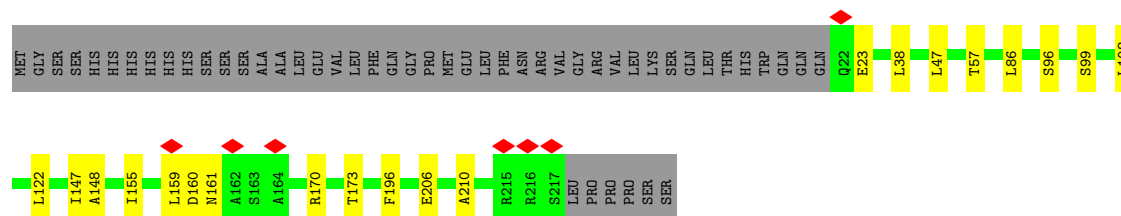
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain p:  73% 7% 20%



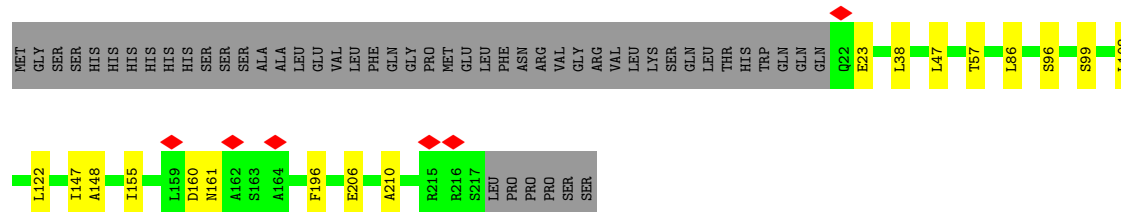
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain q:  72% 8% 20%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain r:  73% 7% 20%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

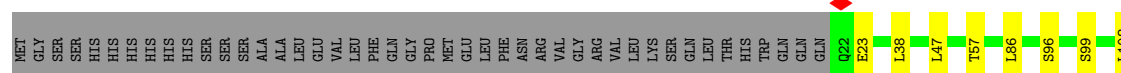
Chain s:  74% 6% 20%





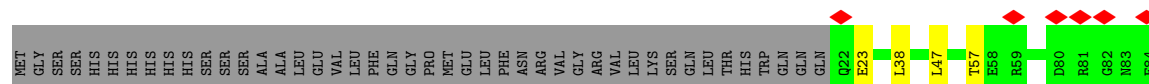
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain t: 73% 7% 20%



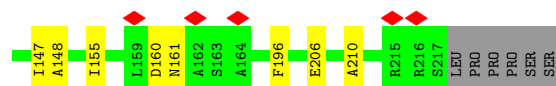
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain u: 9% 74% 6% 20%



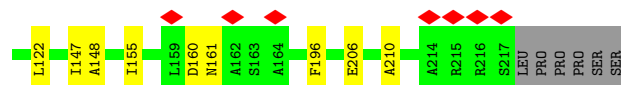
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain v: 74% 6% 20%



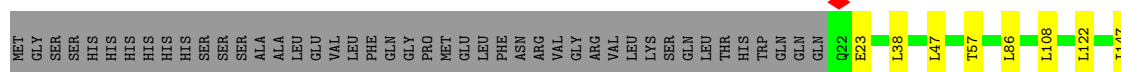
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain w: 73% 7% 20%



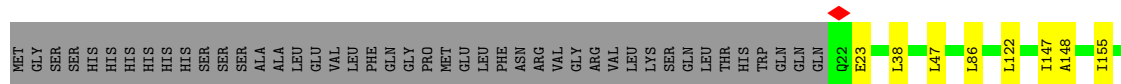
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain x:  74% 6% 20%



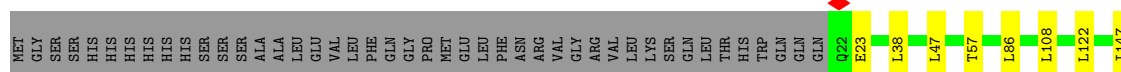
- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain y:  74% 5% 20%



- Molecule 1: Chloroplast membrane-associated 30 kD protein

Chain z:  73% 7% 20%



## 4 Experimental information

| Property                           | Value                                            | Source    |
|------------------------------------|--------------------------------------------------|-----------|
| EM reconstruction method           | HELICAL                                          | Depositor |
| Imposed symmetry                   | HELICAL, twist=130.2°, rise=2.52 Å, axial sym=C1 | Depositor |
| Number of segments used            | 48854                                            | Depositor |
| Resolution determination method    | FSC 0.143 CUT-OFF                                | Depositor |
| CTF correction method              | PHASE FLIPPING AND AMPLITUDE CORRECTION          | Depositor |
| Microscope                         | FEI TALOS ARCTICA                                | Depositor |
| Voltage (kV)                       | 200                                              | Depositor |
| Electron dose ( $e^-/\text{Å}^2$ ) | 58                                               | Depositor |
| Minimum defocus (nm)               | 1000                                             | Depositor |
| Maximum defocus (nm)               | 4000                                             | Depositor |
| Magnification                      | Not provided                                     |           |
| Image detector                     | GATAN K3 BIOQUANTUM (6k x 4k)                    | Depositor |
| Maximum map value                  | 0.674                                            | Depositor |
| Minimum map value                  | -0.330                                           | Depositor |
| Average map value                  | 0.002                                            | Depositor |
| Map value standard deviation       | 0.019                                            | Depositor |
| Recommended contour level          | 0.12                                             | Depositor |
| Map size (Å)                       | 544.8, 544.8, 544.8                              | wwPDB     |
| Map dimensions                     | 400, 400, 400                                    | wwPDB     |
| Map angles (°)                     | 90.0, 90.0, 90.0                                 | wwPDB     |
| Pixel spacing (Å)                  | 1.362, 1.362, 1.362                              | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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   | 0     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | 1     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | 2     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | 3     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | 4     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | 5     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | 6     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | 7     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | A     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | B     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | C     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | D     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | E     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | F     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | G     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | H     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | I     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | J     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | K     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | L     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | M     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | N     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | O     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | P     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | Q     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | R     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | S     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | T     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | U     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | V     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | W     | 0.11         | 0/1593      | 0.20        | 0/2138      |
| 1   | X     | 0.11         | 0/1593      | 0.20        | 0/2138      |

| Mol | Chain | Bond lengths |         | Bond angles |          |
|-----|-------|--------------|---------|-------------|----------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5  |
| 1   | Y     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | Z     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | a     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | b     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | c     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | d     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | e     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | f     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | g     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | h     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | i     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | j     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | k     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | l     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | m     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | n     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | o     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | p     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | q     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | r     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | s     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | t     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | u     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | v     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | w     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | x     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | y     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| 1   | z     | 0.11         | 0/1593  | 0.20        | 0/2138   |
| All | All   | 0.11         | 0/95580 | 0.20        | 0/128280 |

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   | 0     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | 1     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | 2     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | 3     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | 4     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | 5     | 1577  | 190      | 1603     | 12      | 0            |
| 1   | 6     | 1577  | 190      | 1603     | 12      | 0            |
| 1   | 7     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | A     | 1577  | 190      | 1603     | 11      | 0            |
| 1   | B     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | C     | 1577  | 190      | 1603     | 11      | 0            |
| 1   | D     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | E     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | F     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | G     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | H     | 1577  | 190      | 1603     | 12      | 0            |
| 1   | I     | 1577  | 190      | 1603     | 15      | 0            |
| 1   | J     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | K     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | L     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | M     | 1577  | 190      | 1603     | 15      | 0            |
| 1   | N     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | O     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | P     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | Q     | 1577  | 190      | 1603     | 12      | 0            |
| 1   | R     | 1577  | 190      | 1603     | 16      | 0            |
| 1   | S     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | T     | 1577  | 190      | 1603     | 12      | 0            |
| 1   | U     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | V     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | W     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | X     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | Y     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | Z     | 1577  | 190      | 1603     | 12      | 0            |
| 1   | a     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | b     | 1577  | 190      | 1603     | 15      | 0            |
| 1   | c     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | d     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | e     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | f     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | g     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | h     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | i     | 1577  | 190      | 1603     | 14      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | j     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | k     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | l     | 1577  | 190      | 1603     | 15      | 0            |
| 1   | m     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | n     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | o     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | p     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | q     | 1577  | 190      | 1603     | 16      | 0            |
| 1   | r     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | s     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | t     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | u     | 1577  | 190      | 1603     | 12      | 0            |
| 1   | v     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | w     | 1577  | 190      | 1603     | 14      | 0            |
| 1   | x     | 1577  | 190      | 1603     | 13      | 0            |
| 1   | y     | 1577  | 190      | 1603     | 12      | 0            |
| 1   | z     | 1577  | 190      | 1603     | 14      | 0            |
| 2   | 0     | 27    | 0        | 12       | 2       | 0            |
| 2   | 1     | 27    | 0        | 12       | 2       | 0            |
| 2   | 2     | 27    | 0        | 12       | 2       | 0            |
| 2   | 3     | 27    | 0        | 12       | 2       | 0            |
| 2   | 4     | 27    | 0        | 12       | 2       | 0            |
| 2   | 5     | 27    | 0        | 12       | 2       | 0            |
| 2   | 6     | 27    | 0        | 12       | 2       | 0            |
| 2   | 7     | 27    | 0        | 12       | 2       | 0            |
| 2   | A     | 27    | 0        | 12       | 2       | 0            |
| 2   | B     | 27    | 0        | 12       | 2       | 0            |
| 2   | C     | 27    | 0        | 12       | 2       | 0            |
| 2   | D     | 27    | 0        | 12       | 2       | 0            |
| 2   | E     | 27    | 0        | 12       | 2       | 0            |
| 2   | F     | 27    | 0        | 12       | 2       | 0            |
| 2   | G     | 27    | 0        | 12       | 2       | 0            |
| 2   | H     | 27    | 0        | 12       | 2       | 0            |
| 2   | I     | 27    | 0        | 12       | 2       | 0            |
| 2   | J     | 27    | 0        | 12       | 2       | 0            |
| 2   | K     | 27    | 0        | 12       | 2       | 0            |
| 2   | L     | 27    | 0        | 12       | 2       | 0            |
| 2   | M     | 27    | 0        | 12       | 2       | 0            |
| 2   | N     | 27    | 0        | 12       | 2       | 0            |
| 2   | O     | 27    | 0        | 12       | 2       | 0            |
| 2   | P     | 27    | 0        | 12       | 2       | 0            |
| 2   | Q     | 27    | 0        | 12       | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | R     | 27    | 0        | 12       | 2       | 0            |
| 2   | S     | 27    | 0        | 12       | 2       | 0            |
| 2   | T     | 27    | 0        | 12       | 2       | 0            |
| 2   | U     | 27    | 0        | 12       | 2       | 0            |
| 2   | V     | 27    | 0        | 12       | 2       | 0            |
| 2   | W     | 27    | 0        | 12       | 2       | 0            |
| 2   | X     | 27    | 0        | 12       | 2       | 0            |
| 2   | Y     | 27    | 0        | 12       | 2       | 0            |
| 2   | Z     | 27    | 0        | 12       | 2       | 0            |
| 2   | a     | 27    | 0        | 12       | 2       | 0            |
| 2   | b     | 27    | 0        | 12       | 2       | 0            |
| 2   | c     | 27    | 0        | 12       | 2       | 0            |
| 2   | d     | 27    | 0        | 12       | 2       | 0            |
| 2   | e     | 27    | 0        | 12       | 2       | 0            |
| 2   | f     | 27    | 0        | 12       | 2       | 0            |
| 2   | g     | 27    | 0        | 12       | 2       | 0            |
| 2   | h     | 27    | 0        | 12       | 2       | 0            |
| 2   | i     | 27    | 0        | 12       | 2       | 0            |
| 2   | j     | 27    | 0        | 12       | 2       | 0            |
| 2   | k     | 27    | 0        | 12       | 2       | 0            |
| 2   | l     | 27    | 0        | 12       | 2       | 0            |
| 2   | m     | 27    | 0        | 12       | 2       | 0            |
| 2   | n     | 27    | 0        | 12       | 2       | 0            |
| 2   | o     | 27    | 0        | 12       | 2       | 0            |
| 2   | p     | 27    | 0        | 12       | 2       | 0            |
| 2   | q     | 27    | 0        | 12       | 2       | 0            |
| 2   | r     | 27    | 0        | 12       | 2       | 0            |
| 2   | s     | 27    | 0        | 12       | 2       | 0            |
| 2   | t     | 27    | 0        | 12       | 2       | 0            |
| 2   | u     | 27    | 0        | 12       | 2       | 0            |
| 2   | v     | 27    | 0        | 12       | 2       | 0            |
| 2   | w     | 27    | 0        | 12       | 2       | 0            |
| 2   | x     | 27    | 0        | 12       | 2       | 0            |
| 2   | y     | 27    | 0        | 12       | 2       | 0            |
| 2   | z     | 27    | 0        | 12       | 2       | 0            |
| All | All   | 96240 | 11400    | 96900    | 745     | 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 4.

All (745) 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:Q:160:ASP:O | 2:Q:301:ADP:O2' | 1.98                     | 0.82              |
| 1:T:160:ASP:O | 2:T:301:ADP:O2' | 1.98                     | 0.82              |
| 1:Y:160:ASP:O | 2:Y:301:ADP:O2' | 1.98                     | 0.82              |
| 1:b:160:ASP:O | 2:b:301:ADP:O2' | 1.98                     | 0.82              |
| 1:N:160:ASP:O | 2:N:301:ADP:O2' | 1.98                     | 0.82              |
| 1:4:160:ASP:O | 2:4:301:ADP:O2' | 1.98                     | 0.82              |
| 1:I:160:ASP:O | 2:I:301:ADP:O2' | 1.98                     | 0.82              |
| 1:V:160:ASP:O | 2:V:301:ADP:O2' | 1.98                     | 0.82              |
| 1:1:160:ASP:O | 2:1:301:ADP:O2' | 1.98                     | 0.82              |
| 1:W:160:ASP:O | 2:W:301:ADP:O2' | 1.98                     | 0.82              |
| 1:e:160:ASP:O | 2:e:301:ADP:O2' | 1.98                     | 0.82              |
| 1:7:160:ASP:O | 2:7:301:ADP:O2' | 1.98                     | 0.81              |
| 1:F:160:ASP:O | 2:F:301:ADP:O2' | 1.98                     | 0.81              |
| 1:6:160:ASP:O | 2:6:301:ADP:O2' | 1.98                     | 0.81              |
| 1:L:160:ASP:O | 2:L:301:ADP:O2' | 1.98                     | 0.81              |
| 1:j:160:ASP:O | 2:j:301:ADP:O2' | 1.98                     | 0.81              |
| 1:K:160:ASP:O | 2:K:301:ADP:O2' | 1.98                     | 0.81              |
| 1:f:160:ASP:O | 2:f:301:ADP:O2' | 1.98                     | 0.81              |
| 1:g:160:ASP:O | 2:g:301:ADP:O2' | 1.98                     | 0.81              |
| 1:M:160:ASP:O | 2:M:301:ADP:O2' | 1.98                     | 0.81              |
| 1:x:160:ASP:O | 2:x:301:ADP:O2' | 1.98                     | 0.81              |
| 1:B:160:ASP:O | 2:B:301:ADP:O2' | 1.98                     | 0.81              |
| 1:h:160:ASP:O | 2:h:301:ADP:O2' | 1.98                     | 0.81              |
| 1:m:160:ASP:O | 2:m:301:ADP:O2' | 1.98                     | 0.81              |
| 1:y:160:ASP:O | 2:y:301:ADP:O2' | 1.98                     | 0.81              |
| 1:C:160:ASP:O | 2:C:301:ADP:O2' | 1.98                     | 0.81              |
| 1:S:160:ASP:O | 2:S:301:ADP:O2' | 1.98                     | 0.81              |
| 1:Z:160:ASP:O | 2:Z:301:ADP:O2' | 1.98                     | 0.81              |
| 1:q:160:ASP:O | 2:q:301:ADP:O2' | 1.98                     | 0.81              |
| 1:U:160:ASP:O | 2:U:301:ADP:O2' | 1.98                     | 0.81              |
| 1:X:160:ASP:O | 2:X:301:ADP:O2' | 1.98                     | 0.81              |
| 1:3:160:ASP:O | 2:3:301:ADP:O2' | 1.98                     | 0.81              |
| 1:O:160:ASP:O | 2:O:301:ADP:O2' | 1.98                     | 0.81              |
| 1:H:160:ASP:O | 2:H:301:ADP:O2' | 1.98                     | 0.81              |
| 1:s:160:ASP:O | 2:s:301:ADP:O2' | 1.98                     | 0.81              |
| 1:w:160:ASP:O | 2:w:301:ADP:O2' | 1.98                     | 0.81              |
| 1:A:160:ASP:O | 2:A:301:ADP:O2' | 1.98                     | 0.80              |
| 1:d:160:ASP:O | 2:d:301:ADP:O2' | 1.98                     | 0.80              |
| 1:G:160:ASP:O | 2:G:301:ADP:O2' | 1.98                     | 0.80              |
| 1:l:160:ASP:O | 2:l:301:ADP:O2' | 1.98                     | 0.80              |
| 1:p:160:ASP:O | 2:p:301:ADP:O2' | 1.98                     | 0.80              |
| 1:2:160:ASP:O | 2:2:301:ADP:O2' | 1.98                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:k:160:ASP:O    | 2:k:301:ADP:O2'  | 1.98                     | 0.80              |
| 1:v:160:ASP:O    | 2:v:301:ADP:O2'  | 1.98                     | 0.80              |
| 1:c:160:ASP:O    | 2:c:301:ADP:O2'  | 1.98                     | 0.80              |
| 1:u:160:ASP:O    | 2:u:301:ADP:O2'  | 1.98                     | 0.80              |
| 1:5:160:ASP:O    | 2:5:301:ADP:O2'  | 1.98                     | 0.80              |
| 1:J:160:ASP:O    | 2:J:301:ADP:O2'  | 1.98                     | 0.80              |
| 1:P:160:ASP:O    | 2:P:301:ADP:O2'  | 1.98                     | 0.80              |
| 1:0:160:ASP:O    | 2:0:301:ADP:O2'  | 1.98                     | 0.80              |
| 1:r:160:ASP:O    | 2:r:301:ADP:O2'  | 1.98                     | 0.80              |
| 1:E:160:ASP:O    | 2:E:301:ADP:O2'  | 1.98                     | 0.80              |
| 1:i:160:ASP:O    | 2:i:301:ADP:O2'  | 1.98                     | 0.80              |
| 1:z:160:ASP:O    | 2:z:301:ADP:O2'  | 1.98                     | 0.80              |
| 1:D:160:ASP:O    | 2:D:301:ADP:O2'  | 1.98                     | 0.80              |
| 1:n:160:ASP:O    | 2:n:301:ADP:O2'  | 1.98                     | 0.80              |
| 1:R:160:ASP:O    | 2:R:301:ADP:O2'  | 1.98                     | 0.80              |
| 1:o:160:ASP:O    | 2:o:301:ADP:O2'  | 1.98                     | 0.80              |
| 1:a:160:ASP:O    | 2:a:301:ADP:O2'  | 1.98                     | 0.79              |
| 1:t:160:ASP:O    | 2:t:301:ADP:O2'  | 1.98                     | 0.79              |
| 1:F:155:ILE:HG22 | 1:F:155:ILE:O    | 2.03                     | 0.59              |
| 1:l:155:ILE:HG22 | 1:l:155:ILE:O    | 2.03                     | 0.59              |
| 1:B:155:ILE:HG22 | 1:B:155:ILE:O    | 2.03                     | 0.59              |
| 1:T:155:ILE:O    | 1:T:155:ILE:HG22 | 2.03                     | 0.59              |
| 1:U:155:ILE:HG22 | 1:U:155:ILE:O    | 2.03                     | 0.59              |
| 1:h:155:ILE:HG22 | 1:h:155:ILE:O    | 2.03                     | 0.59              |
| 1:i:155:ILE:HG22 | 1:i:155:ILE:O    | 2.03                     | 0.59              |
| 1:2:155:ILE:O    | 1:2:155:ILE:HG22 | 2.03                     | 0.59              |
| 1:r:155:ILE:HG22 | 1:r:155:ILE:O    | 2.03                     | 0.59              |
| 1:A:155:ILE:HG22 | 1:A:155:ILE:O    | 2.03                     | 0.59              |
| 1:P:155:ILE:HG22 | 1:P:155:ILE:O    | 2.03                     | 0.59              |
| 1:V:155:ILE:O    | 1:V:155:ILE:HG22 | 2.03                     | 0.59              |
| 1:m:155:ILE:HG22 | 1:m:155:ILE:O    | 2.03                     | 0.59              |
| 1:n:155:ILE:HG22 | 1:n:155:ILE:O    | 2.03                     | 0.59              |
| 1:x:155:ILE:O    | 1:x:155:ILE:HG22 | 2.03                     | 0.59              |
| 1:G:155:ILE:HG22 | 1:G:155:ILE:O    | 2.03                     | 0.59              |
| 1:O:155:ILE:O    | 1:O:155:ILE:HG22 | 2.03                     | 0.59              |
| 1:Y:155:ILE:O    | 1:Y:155:ILE:HG22 | 2.03                     | 0.59              |
| 1:w:155:ILE:HG22 | 1:w:155:ILE:O    | 2.03                     | 0.59              |
| 1:7:155:ILE:O    | 1:7:155:ILE:HG22 | 2.03                     | 0.59              |
| 1:s:155:ILE:O    | 1:s:155:ILE:HG22 | 2.03                     | 0.59              |
| 1:K:155:ILE:HG22 | 1:K:155:ILE:O    | 2.03                     | 0.59              |
| 1:L:155:ILE:HG22 | 1:L:155:ILE:O    | 2.03                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:155:ILE:HG22 | 1:Z:155:ILE:O    | 2.03                     | 0.59              |
| 1:v:155:ILE:O    | 1:v:155:ILE:HG22 | 2.03                     | 0.59              |
| 1:6:155:ILE:HG22 | 1:6:155:ILE:O    | 2.03                     | 0.59              |
| 1:d:155:ILE:HG22 | 1:d:155:ILE:O    | 2.03                     | 0.59              |
| 1:t:155:ILE:HG22 | 1:t:155:ILE:O    | 2.03                     | 0.59              |
| 1:u:155:ILE:HG22 | 1:u:155:ILE:O    | 2.03                     | 0.59              |
| 1:M:155:ILE:O    | 1:M:155:ILE:HG22 | 2.03                     | 0.59              |
| 1:a:155:ILE:HG22 | 1:a:155:ILE:O    | 2.03                     | 0.59              |
| 1:c:155:ILE:HG22 | 1:c:155:ILE:O    | 2.03                     | 0.59              |
| 1:e:155:ILE:O    | 1:e:155:ILE:HG22 | 2.03                     | 0.59              |
| 1:I:155:ILE:HG22 | 1:I:155:ILE:O    | 2.03                     | 0.58              |
| 1:J:155:ILE:O    | 1:J:155:ILE:HG22 | 2.03                     | 0.58              |
| 1:Q:155:ILE:O    | 1:Q:155:ILE:HG22 | 2.03                     | 0.58              |
| 1:b:155:ILE:O    | 1:b:155:ILE:HG22 | 2.03                     | 0.58              |
| 1:f:155:ILE:HG22 | 1:f:155:ILE:O    | 2.03                     | 0.58              |
| 1:o:155:ILE:O    | 1:o:155:ILE:HG22 | 2.03                     | 0.58              |
| 1:p:155:ILE:HG22 | 1:p:155:ILE:O    | 2.03                     | 0.58              |
| 1:q:155:ILE:O    | 1:q:155:ILE:HG22 | 2.03                     | 0.58              |
| 1:y:155:ILE:HG22 | 1:y:155:ILE:O    | 2.03                     | 0.58              |
| 1:0:155:ILE:HG22 | 1:0:155:ILE:O    | 2.03                     | 0.58              |
| 1:N:155:ILE:HG22 | 1:N:155:ILE:O    | 2.03                     | 0.58              |
| 1:3:155:ILE:HG22 | 1:3:155:ILE:O    | 2.03                     | 0.58              |
| 1:5:155:ILE:HG22 | 1:5:155:ILE:O    | 2.03                     | 0.58              |
| 1:C:155:ILE:O    | 1:C:155:ILE:HG22 | 2.03                     | 0.58              |
| 1:X:155:ILE:HG22 | 1:X:155:ILE:O    | 2.03                     | 0.58              |
| 1:4:155:ILE:O    | 1:4:155:ILE:HG22 | 2.03                     | 0.58              |
| 1:j:155:ILE:O    | 1:j:155:ILE:HG22 | 2.03                     | 0.58              |
| 1:H:155:ILE:O    | 1:H:155:ILE:HG22 | 2.03                     | 0.58              |
| 1:l:155:ILE:O    | 1:l:155:ILE:HG22 | 2.03                     | 0.58              |
| 1:W:155:ILE:HG22 | 1:W:155:ILE:O    | 2.03                     | 0.58              |
| 1:E:155:ILE:O    | 1:E:155:ILE:HG22 | 2.03                     | 0.58              |
| 1:R:155:ILE:HG22 | 1:R:155:ILE:O    | 2.03                     | 0.58              |
| 1:g:155:ILE:O    | 1:g:155:ILE:HG22 | 2.03                     | 0.58              |
| 1:S:155:ILE:HG22 | 1:S:155:ILE:O    | 2.03                     | 0.58              |
| 1:z:155:ILE:HG22 | 1:z:155:ILE:O    | 2.03                     | 0.58              |
| 1:k:155:ILE:HG22 | 1:k:155:ILE:O    | 2.03                     | 0.57              |
| 1:D:155:ILE:HG22 | 1:D:155:ILE:O    | 2.03                     | 0.57              |
| 1:Q:23:GLU:OE1   | 1:Q:23:GLU:N     | 2.39                     | 0.56              |
| 1:V:23:GLU:OE1   | 1:V:23:GLU:N     | 2.39                     | 0.56              |
| 1:Y:23:GLU:OE1   | 1:Y:23:GLU:N     | 2.39                     | 0.56              |
| 1:N:23:GLU:N     | 1:N:23:GLU:OE1   | 2.39                     | 0.56              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:m:23:GLU:N   | 1:m:23:GLU:OE1 | 2.39                     | 0.56              |
| 1:S:23:GLU:N   | 1:S:23:GLU:OE1 | 2.39                     | 0.56              |
| 1:T:23:GLU:OE1 | 1:T:23:GLU:N   | 2.39                     | 0.56              |
| 1:b:23:GLU:OE1 | 1:b:23:GLU:N   | 2.39                     | 0.56              |
| 1:l:23:GLU:N   | 1:l:23:GLU:OE1 | 2.39                     | 0.56              |
| 1:g:23:GLU:OE1 | 1:g:23:GLU:N   | 2.39                     | 0.56              |
| 1:j:23:GLU:OE1 | 1:j:23:GLU:N   | 2.39                     | 0.56              |
| 1:F:23:GLU:N   | 1:F:23:GLU:OE1 | 2.39                     | 0.56              |
| 1:I:23:GLU:N   | 1:I:23:GLU:OE1 | 2.39                     | 0.56              |
| 1:K:23:GLU:N   | 1:K:23:GLU:OE1 | 2.39                     | 0.56              |
| 1:d:23:GLU:N   | 1:d:23:GLU:OE1 | 2.39                     | 0.56              |
| 1:p:23:GLU:N   | 1:p:23:GLU:OE1 | 2.39                     | 0.56              |
| 1:3:23:GLU:N   | 1:3:23:GLU:OE1 | 2.39                     | 0.56              |
| 1:H:23:GLU:OE1 | 1:H:23:GLU:N   | 2.39                     | 0.56              |
| 1:W:23:GLU:N   | 1:W:23:GLU:OE1 | 2.39                     | 0.56              |
| 1:e:23:GLU:OE1 | 1:e:23:GLU:N   | 2.39                     | 0.56              |
| 1:4:23:GLU:OE1 | 1:4:23:GLU:N   | 2.39                     | 0.56              |
| 1:6:23:GLU:N   | 1:6:23:GLU:OE1 | 2.39                     | 0.56              |
| 1:L:23:GLU:N   | 1:L:23:GLU:OE1 | 2.39                     | 0.56              |
| 1:y:23:GLU:N   | 1:y:23:GLU:OE1 | 2.39                     | 0.56              |
| 1:7:23:GLU:N   | 1:7:23:GLU:OE1 | 2.39                     | 0.55              |
| 1:C:23:GLU:OE1 | 1:C:23:GLU:N   | 2.39                     | 0.55              |
| 1:P:23:GLU:N   | 1:P:23:GLU:OE1 | 2.39                     | 0.55              |
| 1:a:23:GLU:N   | 1:a:23:GLU:OE1 | 2.39                     | 0.55              |
| 1:q:23:GLU:OE1 | 1:q:23:GLU:N   | 2.39                     | 0.55              |
| 1:5:23:GLU:N   | 1:5:23:GLU:OE1 | 2.39                     | 0.55              |
| 1:E:23:GLU:OE1 | 1:E:23:GLU:N   | 2.39                     | 0.55              |
| 1:J:23:GLU:OE1 | 1:J:23:GLU:N   | 2.39                     | 0.55              |
| 1:h:23:GLU:N   | 1:h:23:GLU:OE1 | 2.39                     | 0.55              |
| 1:o:23:GLU:OE1 | 1:o:23:GLU:N   | 2.39                     | 0.55              |
| 1:0:23:GLU:N   | 1:0:23:GLU:OE1 | 2.39                     | 0.55              |
| 1:Z:23:GLU:N   | 1:Z:23:GLU:OE1 | 2.39                     | 0.55              |
| 1:t:23:GLU:N   | 1:t:23:GLU:OE1 | 2.39                     | 0.55              |
| 1:2:23:GLU:OE1 | 1:2:23:GLU:N   | 2.39                     | 0.55              |
| 1:O:23:GLU:OE1 | 1:O:23:GLU:N   | 2.39                     | 0.55              |
| 1:c:23:GLU:N   | 1:c:23:GLU:OE1 | 2.39                     | 0.55              |
| 1:n:23:GLU:N   | 1:n:23:GLU:OE1 | 2.39                     | 0.55              |
| 1:r:23:GLU:N   | 1:r:23:GLU:OE1 | 2.39                     | 0.55              |
| 1:G:23:GLU:N   | 1:G:23:GLU:OE1 | 2.39                     | 0.55              |
| 1:M:23:GLU:N   | 1:M:23:GLU:OE1 | 2.39                     | 0.55              |
| 1:X:23:GLU:N   | 1:X:23:GLU:OE1 | 2.39                     | 0.55              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:s:23:GLU:N   | 1:s:23:GLU:OE1  | 2.39                     | 0.55              |
| 1:u:23:GLU:N   | 1:u:23:GLU:OE1  | 2.39                     | 0.55              |
| 1:l:23:GLU:OE1 | 1:l:23:GLU:N    | 2.39                     | 0.55              |
| 1:v:23:GLU:OE1 | 1:v:23:GLU:N    | 2.39                     | 0.55              |
| 1:A:23:GLU:N   | 1:A:23:GLU:OE1  | 2.39                     | 0.55              |
| 1:R:23:GLU:N   | 1:R:23:GLU:OE1  | 2.39                     | 0.55              |
| 1:f:23:GLU:N   | 1:f:23:GLU:OE1  | 2.39                     | 0.55              |
| 1:k:23:GLU:N   | 1:k:23:GLU:OE1  | 2.39                     | 0.55              |
| 1:U:23:GLU:N   | 1:U:23:GLU:OE1  | 2.39                     | 0.55              |
| 1:w:23:GLU:N   | 1:w:23:GLU:OE1  | 2.39                     | 0.55              |
| 1:B:23:GLU:N   | 1:B:23:GLU:OE1  | 2.39                     | 0.54              |
| 1:D:23:GLU:N   | 1:D:23:GLU:OE1  | 2.39                     | 0.54              |
| 1:i:23:GLU:N   | 1:i:23:GLU:OE1  | 2.39                     | 0.54              |
| 1:U:206:GLU:O  | 1:U:210:ALA:N   | 2.35                     | 0.54              |
| 1:z:23:GLU:N   | 1:z:23:GLU:OE1  | 2.39                     | 0.54              |
| 1:x:23:GLU:OE1 | 1:x:23:GLU:N    | 2.39                     | 0.54              |
| 1:W:161:ASN:O  | 2:W:301:ADP:O3' | 2.24                     | 0.54              |
| 1:b:161:ASN:O  | 2:b:301:ADP:O3' | 2.25                     | 0.54              |
| 1:s:206:GLU:O  | 1:s:210:ALA:N   | 2.35                     | 0.54              |
| 1:6:161:ASN:O  | 2:6:301:ADP:O3' | 2.24                     | 0.54              |
| 1:B:161:ASN:O  | 2:B:301:ADP:O3' | 2.25                     | 0.54              |
| 1:E:161:ASN:O  | 2:E:301:ADP:O3' | 2.25                     | 0.54              |
| 1:l:206:GLU:O  | 1:l:210:ALA:N   | 2.35                     | 0.54              |
| 1:a:161:ASN:O  | 2:a:301:ADP:O3' | 2.25                     | 0.54              |
| 1:0:161:ASN:O  | 2:0:301:ADP:O3' | 2.25                     | 0.54              |
| 1:X:161:ASN:O  | 2:X:301:ADP:O3' | 2.25                     | 0.54              |
| 1:s:161:ASN:O  | 2:s:301:ADP:O3' | 2.25                     | 0.54              |
| 1:c:206:GLU:O  | 1:c:210:ALA:N   | 2.35                     | 0.53              |
| 1:d:161:ASN:O  | 2:d:301:ADP:O3' | 2.25                     | 0.53              |
| 1:e:206:GLU:O  | 1:e:210:ALA:N   | 2.35                     | 0.53              |
| 1:x:161:ASN:O  | 2:x:301:ADP:O3' | 2.25                     | 0.53              |
| 1:y:161:ASN:O  | 2:y:301:ADP:O3' | 2.24                     | 0.53              |
| 1:H:161:ASN:O  | 2:H:301:ADP:O3' | 2.25                     | 0.53              |
| 1:k:206:GLU:O  | 1:k:210:ALA:N   | 2.35                     | 0.53              |
| 1:t:161:ASN:O  | 2:t:301:ADP:O3' | 2.25                     | 0.53              |
| 1:t:206:GLU:O  | 1:t:210:ALA:N   | 2.35                     | 0.53              |
| 1:3:161:ASN:O  | 2:3:301:ADP:O3' | 2.25                     | 0.53              |
| 1:U:161:ASN:O  | 2:U:301:ADP:O3' | 2.25                     | 0.53              |
| 1:T:161:ASN:O  | 2:T:301:ADP:O3' | 2.25                     | 0.53              |
| 1:d:206:GLU:O  | 1:d:210:ALA:N   | 2.35                     | 0.53              |
| 1:Q:206:GLU:O  | 1:Q:210:ALA:N   | 2.35                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:g:161:ASN:O    | 2:g:301:ADP:O3'  | 2.25                     | 0.53              |
| 1:q:161:ASN:O    | 2:q:301:ADP:O3'  | 2.25                     | 0.53              |
| 1:Y:161:ASN:O    | 2:Y:301:ADP:O3'  | 2.24                     | 0.53              |
| 1:R:161:ASN:O    | 2:R:301:ADP:O3'  | 2.25                     | 0.53              |
| 1:G:206:GLU:O    | 1:G:210:ALA:N    | 2.35                     | 0.52              |
| 1:K:161:ASN:O    | 2:K:301:ADP:O3'  | 2.24                     | 0.52              |
| 1:n:161:ASN:O    | 2:n:301:ADP:O3'  | 2.24                     | 0.52              |
| 1:2:206:GLU:O    | 1:2:210:ALA:N    | 2.35                     | 0.52              |
| 1:C:206:GLU:O    | 1:C:210:ALA:N    | 2.35                     | 0.52              |
| 1:J:161:ASN:O    | 2:J:301:ADP:O3'  | 2.25                     | 0.52              |
| 1:O:161:ASN:O    | 2:O:301:ADP:O3'  | 2.24                     | 0.52              |
| 1:5:161:ASN:O    | 2:5:301:ADP:O3'  | 2.25                     | 0.52              |
| 1:Q:122:LEU:HD23 | 1:Q:122:LEU:C    | 2.35                     | 0.52              |
| 1:W:206:GLU:O    | 1:W:210:ALA:N    | 2.35                     | 0.52              |
| 1:Y:122:LEU:C    | 1:Y:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:m:122:LEU:C    | 1:m:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:p:161:ASN:O    | 2:p:301:ADP:O3'  | 2.25                     | 0.52              |
| 1:1:122:LEU:C    | 1:1:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:G:122:LEU:C    | 1:G:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:N:122:LEU:C    | 1:N:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:U:122:LEU:C    | 1:U:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:a:122:LEU:C    | 1:a:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:l:122:LEU:HD23 | 1:l:122:LEU:C    | 2.35                     | 0.52              |
| 1:n:122:LEU:C    | 1:n:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:2:122:LEU:HD23 | 1:2:122:LEU:C    | 2.35                     | 0.52              |
| 1:5:122:LEU:C    | 1:5:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:7:122:LEU:C    | 1:7:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:F:122:LEU:C    | 1:F:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:J:122:LEU:HD23 | 1:J:122:LEU:C    | 2.35                     | 0.52              |
| 1:K:122:LEU:C    | 1:K:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:M:122:LEU:C    | 1:M:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:S:122:LEU:C    | 1:S:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:X:206:GLU:O    | 1:X:210:ALA:N    | 2.35                     | 0.52              |
| 1:Z:47:LEU:C     | 1:Z:47:LEU:HD23  | 2.35                     | 0.52              |
| 1:i:122:LEU:C    | 1:i:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:j:122:LEU:C    | 1:j:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:p:122:LEU:C    | 1:p:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:s:122:LEU:HD23 | 1:s:122:LEU:C    | 2.35                     | 0.52              |
| 1:y:206:GLU:O    | 1:y:210:ALA:N    | 2.35                     | 0.52              |
| 1:6:122:LEU:C    | 1:6:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:A:47:LEU:C     | 1:A:47:LEU:HD23  | 2.35                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:122:LEU:HD23 | 1:E:122:LEU:C    | 2.35                     | 0.52              |
| 1:I:47:LEU:C     | 1:I:47:LEU:HD23  | 2.35                     | 0.52              |
| 1:L:122:LEU:C    | 1:L:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:P:206:GLU:O    | 1:P:210:ALA:N    | 2.35                     | 0.52              |
| 1:T:122:LEU:HD23 | 1:T:122:LEU:C    | 2.35                     | 0.52              |
| 1:Z:122:LEU:C    | 1:Z:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:e:122:LEU:HD23 | 1:e:122:LEU:C    | 2.35                     | 0.52              |
| 1:f:122:LEU:C    | 1:f:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:g:122:LEU:HD23 | 1:g:122:LEU:C    | 2.35                     | 0.52              |
| 1:h:47:LEU:C     | 1:h:47:LEU:HD23  | 2.35                     | 0.52              |
| 1:k:161:ASN:O    | 2:k:301:ADP:O3'  | 2.24                     | 0.52              |
| 1:n:47:LEU:C     | 1:n:47:LEU:HD23  | 2.35                     | 0.52              |
| 1:o:122:LEU:C    | 1:o:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:w:47:LEU:C     | 1:w:47:LEU:HD23  | 2.35                     | 0.52              |
| 1:1:161:ASN:O    | 2:1:301:ADP:O3'  | 2.25                     | 0.52              |
| 1:4:47:LEU:HD23  | 1:4:47:LEU:C     | 2.35                     | 0.52              |
| 1:C:122:LEU:HD23 | 1:C:122:LEU:C    | 2.35                     | 0.52              |
| 1:L:161:ASN:O    | 2:L:301:ADP:O3'  | 2.25                     | 0.52              |
| 1:O:206:GLU:O    | 1:O:210:ALA:N    | 2.35                     | 0.52              |
| 1:P:122:LEU:C    | 1:P:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:R:47:LEU:C     | 1:R:47:LEU:HD23  | 2.35                     | 0.52              |
| 1:k:47:LEU:C     | 1:k:47:LEU:HD23  | 2.35                     | 0.52              |
| 1:s:47:LEU:C     | 1:s:47:LEU:HD23  | 2.35                     | 0.52              |
| 1:t:122:LEU:C    | 1:t:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:v:122:LEU:HD23 | 1:v:122:LEU:C    | 2.35                     | 0.52              |
| 1:x:122:LEU:HD23 | 1:x:122:LEU:C    | 2.35                     | 0.52              |
| 1:0:122:LEU:C    | 1:0:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:7:47:LEU:C     | 1:7:47:LEU:HD23  | 2.35                     | 0.52              |
| 1:B:122:LEU:C    | 1:B:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:D:122:LEU:C    | 1:D:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:W:122:LEU:C    | 1:W:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:e:161:ASN:O    | 2:e:301:ADP:O3'  | 2.25                     | 0.52              |
| 1:h:122:LEU:C    | 1:h:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:j:161:ASN:O    | 2:j:301:ADP:O3'  | 2.24                     | 0.52              |
| 1:p:47:LEU:C     | 1:p:47:LEU:HD23  | 2.35                     | 0.52              |
| 1:u:122:LEU:C    | 1:u:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:u:161:ASN:O    | 2:u:301:ADP:O3'  | 2.25                     | 0.52              |
| 1:y:122:LEU:C    | 1:y:122:LEU:HD23 | 2.35                     | 0.52              |
| 1:3:47:LEU:C     | 1:3:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:7:161:ASN:O    | 2:7:301:ADP:O3'  | 2.25                     | 0.51              |
| 1:A:122:LEU:C    | 1:A:122:LEU:HD23 | 2.35                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:47:LEU:HD23  | 1:H:47:LEU:C     | 2.35                     | 0.51              |
| 1:O:47:LEU:HD23  | 1:O:47:LEU:C     | 2.35                     | 0.51              |
| 1:P:47:LEU:C     | 1:P:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:T:47:LEU:HD23  | 1:T:47:LEU:C     | 2.35                     | 0.51              |
| 1:a:47:LEU:C     | 1:a:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:c:122:LEU:C    | 1:c:122:LEU:HD23 | 2.35                     | 0.51              |
| 1:f:47:LEU:C     | 1:f:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:h:161:ASN:O    | 2:h:301:ADP:O3'  | 2.24                     | 0.51              |
| 1:r:47:LEU:C     | 1:r:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:w:122:LEU:C    | 1:w:122:LEU:HD23 | 2.35                     | 0.51              |
| 1:z:47:LEU:C     | 1:z:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:z:122:LEU:C    | 1:z:122:LEU:HD23 | 2.35                     | 0.51              |
| 1:3:122:LEU:C    | 1:3:122:LEU:HD23 | 2.35                     | 0.51              |
| 1:4:161:ASN:O    | 2:4:301:ADP:O3'  | 2.24                     | 0.51              |
| 1:D:47:LEU:C     | 1:D:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:I:161:ASN:O    | 2:I:301:ADP:O3'  | 2.25                     | 0.51              |
| 1:L:47:LEU:C     | 1:L:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:O:122:LEU:HD23 | 1:O:122:LEU:C    | 2.35                     | 0.51              |
| 1:Q:47:LEU:C     | 1:Q:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:j:206:GLU:O    | 1:j:210:ALA:N    | 2.35                     | 0.51              |
| 1:5:47:LEU:C     | 1:5:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:E:47:LEU:HD23  | 1:E:47:LEU:C     | 2.35                     | 0.51              |
| 1:G:47:LEU:C     | 1:G:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:H:122:LEU:C    | 1:H:122:LEU:HD23 | 2.35                     | 0.51              |
| 1:J:47:LEU:HD23  | 1:J:47:LEU:C     | 2.35                     | 0.51              |
| 1:W:47:LEU:C     | 1:W:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:q:47:LEU:HD23  | 1:q:47:LEU:C     | 2.35                     | 0.51              |
| 1:q:122:LEU:HD23 | 1:q:122:LEU:C    | 2.35                     | 0.51              |
| 1:r:122:LEU:C    | 1:r:122:LEU:HD23 | 2.35                     | 0.51              |
| 1:C:47:LEU:HD23  | 1:C:47:LEU:C     | 2.35                     | 0.51              |
| 1:F:47:LEU:C     | 1:F:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:Q:161:ASN:O    | 2:Q:301:ADP:O3'  | 2.25                     | 0.51              |
| 1:R:122:LEU:C    | 1:R:122:LEU:HD23 | 2.35                     | 0.51              |
| 1:g:47:LEU:C     | 1:g:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:v:161:ASN:O    | 2:v:301:ADP:O3'  | 2.24                     | 0.51              |
| 1:y:47:LEU:C     | 1:y:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:1:47:LEU:C     | 1:1:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:2:47:LEU:HD23  | 1:2:47:LEU:C     | 2.35                     | 0.51              |
| 1:S:47:LEU:C     | 1:S:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:c:47:LEU:C     | 1:c:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:e:47:LEU:HD23  | 1:e:47:LEU:C     | 2.35                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:0:47:LEU:C     | 1:0:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:G:161:ASN:O    | 2:G:301:ADP:O3'  | 2.25                     | 0.51              |
| 1:b:47:LEU:C     | 1:b:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:b:122:LEU:HD23 | 1:b:122:LEU:C    | 2.35                     | 0.51              |
| 1:l:47:LEU:HD23  | 1:l:47:LEU:C     | 2.35                     | 0.51              |
| 1:N:161:ASN:O    | 2:N:301:ADP:O3'  | 2.24                     | 0.51              |
| 1:X:47:LEU:C     | 1:X:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:X:122:LEU:C    | 1:X:122:LEU:HD23 | 2.35                     | 0.51              |
| 1:Y:47:LEU:HD23  | 1:Y:47:LEU:C     | 2.35                     | 0.51              |
| 1:d:47:LEU:C     | 1:d:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:d:122:LEU:C    | 1:d:122:LEU:HD23 | 2.35                     | 0.51              |
| 1:f:206:GLU:O    | 1:f:210:ALA:N    | 2.35                     | 0.51              |
| 1:B:47:LEU:C     | 1:B:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:V:122:LEU:HD23 | 1:V:122:LEU:C    | 2.35                     | 0.51              |
| 1:j:47:LEU:HD23  | 1:j:47:LEU:C     | 2.35                     | 0.51              |
| 1:2:161:ASN:O    | 2:2:301:ADP:O3'  | 2.25                     | 0.51              |
| 1:7:38:LEU:C     | 1:7:38:LEU:HD13  | 2.36                     | 0.51              |
| 1:I:206:GLU:O    | 1:I:210:ALA:N    | 2.35                     | 0.51              |
| 1:N:47:LEU:C     | 1:N:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:T:38:LEU:C     | 1:T:38:LEU:HD13  | 2.36                     | 0.51              |
| 1:V:47:LEU:C     | 1:V:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:V:206:GLU:O    | 1:V:210:ALA:N    | 2.35                     | 0.51              |
| 1:e:38:LEU:C     | 1:e:38:LEU:HD13  | 2.36                     | 0.51              |
| 1:i:47:LEU:C     | 1:i:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:k:122:LEU:C    | 1:k:122:LEU:HD23 | 2.35                     | 0.51              |
| 1:o:47:LEU:HD23  | 1:o:47:LEU:C     | 2.35                     | 0.51              |
| 1:p:38:LEU:HD13  | 1:p:38:LEU:C     | 2.36                     | 0.51              |
| 1:x:47:LEU:C     | 1:x:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:z:38:LEU:HD13  | 1:z:38:LEU:C     | 2.36                     | 0.51              |
| 1:4:206:GLU:O    | 1:4:210:ALA:N    | 2.35                     | 0.51              |
| 1:5:38:LEU:C     | 1:5:38:LEU:HD13  | 2.36                     | 0.51              |
| 1:6:47:LEU:C     | 1:6:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:J:38:LEU:HD13  | 1:J:38:LEU:C     | 2.36                     | 0.51              |
| 1:L:38:LEU:HD13  | 1:L:38:LEU:C     | 2.36                     | 0.51              |
| 1:R:38:LEU:C     | 1:R:38:LEU:HD13  | 2.36                     | 0.51              |
| 1:Z:38:LEU:HD13  | 1:Z:38:LEU:C     | 2.36                     | 0.51              |
| 1:h:38:LEU:C     | 1:h:38:LEU:HD13  | 2.36                     | 0.51              |
| 1:i:38:LEU:HD13  | 1:i:38:LEU:C     | 2.36                     | 0.51              |
| 1:m:47:LEU:C     | 1:m:47:LEU:HD23  | 2.35                     | 0.51              |
| 1:q:38:LEU:HD13  | 1:q:38:LEU:C     | 2.36                     | 0.51              |
| 1:4:122:LEU:HD23 | 1:4:122:LEU:C    | 2.35                     | 0.50              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:38:LEU:HD13 | 1:B:38:LEU:C     | 2.36                     | 0.50              |
| 1:D:38:LEU:HD13 | 1:D:38:LEU:C     | 2.36                     | 0.50              |
| 1:W:38:LEU:C    | 1:W:38:LEU:HD13  | 2.36                     | 0.50              |
| 1:X:38:LEU:HD13 | 1:X:38:LEU:C     | 2.36                     | 0.50              |
| 1:b:38:LEU:HD13 | 1:b:38:LEU:C     | 2.36                     | 0.50              |
| 1:f:38:LEU:C    | 1:f:38:LEU:HD13  | 2.36                     | 0.50              |
| 1:t:47:LEU:C    | 1:t:47:LEU:HD23  | 2.35                     | 0.50              |
| 1:u:47:LEU:C    | 1:u:47:LEU:HD23  | 2.35                     | 0.50              |
| 1:v:47:LEU:HD23 | 1:v:47:LEU:C     | 2.35                     | 0.50              |
| 1:x:38:LEU:HD13 | 1:x:38:LEU:C     | 2.36                     | 0.50              |
| 1:1:38:LEU:HD13 | 1:1:38:LEU:C     | 2.36                     | 0.50              |
| 1:2:38:LEU:C    | 1:2:38:LEU:HD13  | 2.36                     | 0.50              |
| 1:6:38:LEU:HD13 | 1:6:38:LEU:C     | 2.36                     | 0.50              |
| 1:C:38:LEU:C    | 1:C:38:LEU:HD13  | 2.36                     | 0.50              |
| 1:I:122:LEU:C   | 1:I:122:LEU:HD23 | 2.35                     | 0.50              |
| 1:K:47:LEU:C    | 1:K:47:LEU:HD23  | 2.35                     | 0.50              |
| 1:S:38:LEU:HD13 | 1:S:38:LEU:C     | 2.36                     | 0.50              |
| 1:a:38:LEU:C    | 1:a:38:LEU:HD13  | 2.36                     | 0.50              |
| 1:m:38:LEU:C    | 1:m:38:LEU:HD13  | 2.36                     | 0.50              |
| 1:y:38:LEU:C    | 1:y:38:LEU:HD13  | 2.36                     | 0.50              |
| 1:K:38:LEU:C    | 1:K:38:LEU:HD13  | 2.36                     | 0.50              |
| 1:O:38:LEU:HD13 | 1:O:38:LEU:C     | 2.36                     | 0.50              |
| 1:j:38:LEU:C    | 1:j:38:LEU:HD13  | 2.36                     | 0.50              |
| 1:s:38:LEU:HD13 | 1:s:38:LEU:C     | 2.36                     | 0.50              |
| 1:0:38:LEU:C    | 1:0:38:LEU:HD13  | 2.36                     | 0.50              |
| 1:A:38:LEU:C    | 1:A:38:LEU:HD13  | 2.36                     | 0.50              |
| 1:F:38:LEU:C    | 1:F:38:LEU:HD13  | 2.36                     | 0.50              |
| 1:G:38:LEU:HD13 | 1:G:38:LEU:C     | 2.36                     | 0.50              |
| 1:M:38:LEU:C    | 1:M:38:LEU:HD13  | 2.36                     | 0.50              |
| 1:U:38:LEU:HD13 | 1:U:38:LEU:C     | 2.36                     | 0.50              |
| 1:c:38:LEU:C    | 1:c:38:LEU:HD13  | 2.36                     | 0.50              |
| 1:n:38:LEU:HD13 | 1:n:38:LEU:C     | 2.36                     | 0.50              |
| 1:t:38:LEU:C    | 1:t:38:LEU:HD13  | 2.36                     | 0.50              |
| 1:B:206:GLU:O   | 1:B:210:ALA:N    | 2.35                     | 0.50              |
| 1:I:38:LEU:HD13 | 1:I:38:LEU:C     | 2.36                     | 0.50              |
| 1:K:206:GLU:O   | 1:K:210:ALA:N    | 2.35                     | 0.50              |
| 1:P:38:LEU:C    | 1:P:38:LEU:HD13  | 2.36                     | 0.50              |
| 1:Q:38:LEU:HD13 | 1:Q:38:LEU:C     | 2.36                     | 0.50              |
| 1:U:47:LEU:C    | 1:U:47:LEU:HD23  | 2.35                     | 0.50              |
| 1:g:206:GLU:O   | 1:g:210:ALA:N    | 2.35                     | 0.50              |
| 1:k:38:LEU:HD13 | 1:k:38:LEU:C     | 2.37                     | 0.50              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:o:38:LEU:C    | 1:o:38:LEU:HD13 | 2.36                     | 0.50              |
| 1:4:38:LEU:HD13 | 1:4:38:LEU:C    | 2.36                     | 0.50              |
| 1:6:206:GLU:O   | 1:6:210:ALA:N   | 2.35                     | 0.50              |
| 1:E:38:LEU:HD13 | 1:E:38:LEU:C    | 2.36                     | 0.50              |
| 1:H:206:GLU:O   | 1:H:210:ALA:N   | 2.35                     | 0.50              |
| 1:N:38:LEU:HD13 | 1:N:38:LEU:C    | 2.36                     | 0.50              |
| 1:Y:38:LEU:C    | 1:Y:38:LEU:HD13 | 2.36                     | 0.50              |
| 1:m:161:ASN:O   | 2:m:301:ADP:O3' | 2.25                     | 0.50              |
| 1:n:206:GLU:O   | 1:n:210:ALA:N   | 2.35                     | 0.50              |
| 1:r:38:LEU:C    | 1:r:38:LEU:HD13 | 2.36                     | 0.50              |
| 1:u:38:LEU:HD13 | 1:u:38:LEU:C    | 2.36                     | 0.50              |
| 1:v:38:LEU:HD13 | 1:v:38:LEU:C    | 2.36                     | 0.50              |
| 1:A:206:GLU:O   | 1:A:210:ALA:N   | 2.35                     | 0.50              |
| 1:V:161:ASN:O   | 2:V:301:ADP:O3' | 2.24                     | 0.50              |
| 1:g:38:LEU:HD13 | 1:g:38:LEU:C    | 2.36                     | 0.50              |
| 1:w:38:LEU:C    | 1:w:38:LEU:HD13 | 2.36                     | 0.50              |
| 1:M:47:LEU:C    | 1:M:47:LEU:HD23 | 2.35                     | 0.50              |
| 1:c:161:ASN:O   | 2:c:301:ADP:O3' | 2.25                     | 0.50              |
| 1:H:38:LEU:C    | 1:H:38:LEU:HD13 | 2.36                     | 0.50              |
| 1:l:38:LEU:HD13 | 1:l:38:LEU:C    | 2.36                     | 0.50              |
| 1:x:206:GLU:O   | 1:x:210:ALA:N   | 2.35                     | 0.50              |
| 1:3:38:LEU:HD13 | 1:3:38:LEU:C    | 2.36                     | 0.49              |
| 1:3:206:GLU:O   | 1:3:210:ALA:N   | 2.35                     | 0.49              |
| 1:J:206:GLU:O   | 1:J:210:ALA:N   | 2.35                     | 0.49              |
| 1:P:161:ASN:O   | 2:P:301:ADP:O3' | 2.25                     | 0.49              |
| 1:V:38:LEU:HD13 | 1:V:38:LEU:C    | 2.36                     | 0.49              |
| 1:w:206:GLU:O   | 1:w:210:ALA:N   | 2.35                     | 0.49              |
| 1:b:206:GLU:O   | 1:b:210:ALA:N   | 2.35                     | 0.49              |
| 1:p:206:GLU:O   | 1:p:210:ALA:N   | 2.35                     | 0.49              |
| 1:l:161:ASN:O   | 2:l:301:ADP:O3' | 2.25                     | 0.49              |
| 1:5:206:GLU:O   | 1:5:210:ALA:N   | 2.35                     | 0.49              |
| 1:M:161:ASN:O   | 2:M:301:ADP:O3' | 2.25                     | 0.49              |
| 1:N:206:GLU:O   | 1:N:210:ALA:N   | 2.35                     | 0.49              |
| 1:S:161:ASN:O   | 2:S:301:ADP:O3' | 2.25                     | 0.49              |
| 1:d:38:LEU:HD13 | 1:d:38:LEU:C    | 2.36                     | 0.49              |
| 1:o:161:ASN:O   | 2:o:301:ADP:O3' | 2.25                     | 0.49              |
| 1:D:161:ASN:O   | 2:D:301:ADP:O3' | 2.24                     | 0.49              |
| 1:i:161:ASN:O   | 2:i:301:ADP:O3' | 2.25                     | 0.49              |
| 1:1:206:GLU:O   | 1:1:210:ALA:N   | 2.35                     | 0.49              |
| 1:F:206:GLU:O   | 1:F:210:ALA:N   | 2.35                     | 0.49              |
| 1:o:206:GLU:O   | 1:o:210:ALA:N   | 2.35                     | 0.48              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:m:206:GLU:O   | 1:m:210:ALA:N   | 2.35                     | 0.48              |
| 1:r:161:ASN:O   | 2:r:301:ADP:O3' | 2.25                     | 0.48              |
| 1:R:206:GLU:O   | 1:R:210:ALA:N   | 2.35                     | 0.48              |
| 1:z:161:ASN:O   | 2:z:301:ADP:O3' | 2.24                     | 0.48              |
| 1:E:206:GLU:O   | 1:E:210:ALA:N   | 2.35                     | 0.48              |
| 1:S:206:GLU:O   | 1:S:210:ALA:N   | 2.35                     | 0.48              |
| 1:r:206:GLU:O   | 1:r:210:ALA:N   | 2.35                     | 0.48              |
| 1:0:206:GLU:O   | 1:0:210:ALA:N   | 2.35                     | 0.48              |
| 1:f:161:ASN:O   | 2:f:301:ADP:O3' | 2.25                     | 0.48              |
| 1:h:206:GLU:O   | 1:h:210:ALA:N   | 2.35                     | 0.48              |
| 1:u:206:GLU:O   | 1:u:210:ALA:N   | 2.35                     | 0.48              |
| 1:A:161:ASN:O   | 2:A:301:ADP:O3' | 2.24                     | 0.48              |
| 1:v:206:GLU:O   | 1:v:210:ALA:N   | 2.35                     | 0.48              |
| 1:Z:161:ASN:O   | 2:Z:301:ADP:O3' | 2.24                     | 0.47              |
| 1:Z:206:GLU:O   | 1:Z:210:ALA:N   | 2.35                     | 0.47              |
| 1:i:206:GLU:O   | 1:i:210:ALA:N   | 2.35                     | 0.47              |
| 1:w:161:ASN:O   | 2:w:301:ADP:O3' | 2.24                     | 0.47              |
| 1:a:206:GLU:O   | 1:a:210:ALA:N   | 2.35                     | 0.47              |
| 1:l:96:SER:O    | 1:l:99:SER:OG   | 2.30                     | 0.47              |
| 1:Y:206:GLU:O   | 1:Y:210:ALA:N   | 2.35                     | 0.47              |
| 1:6:96:SER:O    | 1:6:99:SER:OG   | 2.30                     | 0.47              |
| 1:K:96:SER:O    | 1:K:99:SER:OG   | 2.30                     | 0.47              |
| 1:R:96:SER:O    | 1:R:99:SER:OG   | 2.30                     | 0.47              |
| 1:q:206:GLU:O   | 1:q:210:ALA:N   | 2.35                     | 0.46              |
| 1:T:206:GLU:O   | 1:T:210:ALA:N   | 2.35                     | 0.46              |
| 1:F:161:ASN:O   | 2:F:301:ADP:O3' | 2.25                     | 0.46              |
| 1:e:96:SER:O    | 1:e:99:SER:OG   | 2.30                     | 0.46              |
| 1:r:96:SER:O    | 1:r:99:SER:OG   | 2.30                     | 0.46              |
| 1:3:96:SER:O    | 1:3:99:SER:OG   | 2.30                     | 0.46              |
| 1:C:161:ASN:O   | 2:C:301:ADP:O3' | 2.25                     | 0.46              |
| 1:D:206:GLU:O   | 1:D:210:ALA:N   | 2.35                     | 0.46              |
| 1:3:196:PHE:HE1 | 1:5:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:p:96:SER:O    | 1:p:99:SER:OG   | 2.30                     | 0.45              |
| 1:H:196:PHE:HE1 | 1:J:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:M:206:GLU:O   | 1:M:210:ALA:N   | 2.35                     | 0.45              |
| 1:V:196:PHE:HE1 | 1:X:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:L:206:GLU:O   | 1:L:210:ALA:N   | 2.35                     | 0.45              |
| 1:N:196:PHE:HE1 | 1:P:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:P:196:PHE:HE1 | 1:R:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:o:196:PHE:HE1 | 1:q:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:r:196:PHE:HE1 | 1:t:86:LEU:HD11 | 1.82                     | 0.45              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:t:96:SER:O    | 1:t:99:SER:OG   | 2.30                     | 0.45              |
| 1:v:196:PHE:HE1 | 1:x:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:x:196:PHE:HE1 | 1:z:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:B:86:LEU:HD11 | 1:u:196:PHE:HE1 | 1.82                     | 0.45              |
| 1:B:196:PHE:HE1 | 1:D:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:S:196:PHE:HE1 | 1:U:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:d:196:PHE:HE1 | 1:f:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:z:206:GLU:O   | 1:z:210:ALA:N   | 2.35                     | 0.45              |
| 1:X:196:PHE:HE1 | 1:Z:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:m:196:PHE:HE1 | 1:o:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:1:96:SER:O    | 1:1:99:SER:OG   | 2.30                     | 0.45              |
| 1:M:196:PHE:HE1 | 1:O:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:Q:196:PHE:HE1 | 1:S:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:g:196:PHE:HE1 | 1:i:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:j:196:PHE:HE1 | 1:l:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:l:196:PHE:HE1 | 1:n:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:o:96:SER:O    | 1:o:99:SER:OG   | 2.30                     | 0.45              |
| 1:1:196:PHE:HE1 | 1:3:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:7:206:GLU:O   | 1:7:210:ALA:N   | 2.35                     | 0.45              |
| 1:F:96:SER:O    | 1:F:99:SER:OG   | 2.30                     | 0.45              |
| 1:J:196:PHE:HE1 | 1:L:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:K:196:PHE:HE1 | 1:M:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:b:196:PHE:HE1 | 1:d:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:g:96:SER:O    | 1:g:99:SER:OG   | 2.30                     | 0.45              |
| 1:j:96:SER:O    | 1:j:99:SER:OG   | 2.30                     | 0.45              |
| 1:5:196:PHE:HE1 | 1:7:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:F:196:PHE:HE1 | 1:H:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:Y:196:PHE:HE1 | 1:a:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:h:96:SER:O    | 1:h:99:SER:OG   | 2.30                     | 0.45              |
| 1:t:196:PHE:HE1 | 1:w:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:E:96:SER:O    | 1:E:99:SER:OG   | 2.30                     | 0.45              |
| 1:U:196:PHE:HE1 | 1:W:86:LEU:HD11 | 1.82                     | 0.45              |
| 1:i:196:PHE:HE1 | 1:k:86:LEU:HD11 | 1.82                     | 0.44              |
| 1:p:196:PHE:HE1 | 1:r:86:LEU:HD11 | 1.82                     | 0.44              |
| 1:0:96:SER:O    | 1:0:99:SER:OG   | 2.30                     | 0.44              |
| 1:T:196:PHE:HE1 | 1:V:86:LEU:HD11 | 1.82                     | 0.44              |
| 1:q:196:PHE:HE1 | 1:s:86:LEU:HD11 | 1.82                     | 0.44              |
| 1:M:96:SER:O    | 1:M:99:SER:OG   | 2.30                     | 0.44              |
| 1:a:196:PHE:HE1 | 1:c:86:LEU:HD11 | 1.82                     | 0.44              |
| 1:0:86:LEU:HD11 | 1:y:196:PHE:HE1 | 1.82                     | 0.44              |
| 1:0:196:PHE:HE1 | 1:2:86:LEU:HD11 | 1.82                     | 0.44              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:R:196:PHE:HE1 | 1:T:86:LEU:HD11 | 1.82                     | 0.44              |
| 1:f:196:PHE:HE1 | 1:h:86:LEU:HD11 | 1.82                     | 0.44              |
| 1:s:196:PHE:HE1 | 1:v:86:LEU:HD11 | 1.82                     | 0.44              |
| 1:C:196:PHE:HE1 | 1:E:86:LEU:HD11 | 1.82                     | 0.44              |
| 1:d:96:SER:O    | 1:d:99:SER:OG   | 2.30                     | 0.44              |
| 1:n:196:PHE:HE1 | 1:p:86:LEU:HD11 | 1.82                     | 0.44              |
| 1:E:196:PHE:HE1 | 1:G:86:LEU:HD11 | 1.82                     | 0.44              |
| 1:l:86:LEU:HD11 | 1:z:196:PHE:HE1 | 1.82                     | 0.44              |
| 1:D:196:PHE:HE1 | 1:F:86:LEU:HD11 | 1.82                     | 0.44              |
| 1:L:196:PHE:HE1 | 1:N:86:LEU:HD11 | 1.82                     | 0.44              |
| 1:O:196:PHE:HE1 | 1:Q:86:LEU:HD11 | 1.82                     | 0.44              |
| 1:W:196:PHE:HE1 | 1:Y:86:LEU:HD11 | 1.82                     | 0.44              |
| 1:Z:196:PHE:HE1 | 1:b:86:LEU:HD11 | 1.81                     | 0.44              |
| 1:e:196:PHE:HE1 | 1:g:86:LEU:HD11 | 1.82                     | 0.44              |
| 1:k:196:PHE:HE1 | 1:m:86:LEU:HD11 | 1.82                     | 0.44              |
| 1:m:96:SER:O    | 1:m:99:SER:OG   | 2.30                     | 0.44              |
| 1:l:47:LEU:HD23 | 1:l:47:LEU:O    | 2.18                     | 0.43              |
| 1:E:47:LEU:HD23 | 1:E:47:LEU:O    | 2.18                     | 0.43              |
| 1:F:47:LEU:HD23 | 1:F:47:LEU:O    | 2.18                     | 0.43              |
| 1:N:47:LEU:HD23 | 1:N:47:LEU:O    | 2.18                     | 0.43              |
| 1:d:47:LEU:HD23 | 1:d:47:LEU:O    | 2.18                     | 0.43              |
| 1:h:196:PHE:HE1 | 1:j:86:LEU:HD11 | 1.82                     | 0.43              |
| 1:0:47:LEU:HD23 | 1:0:47:LEU:O    | 2.19                     | 0.43              |
| 1:M:47:LEU:HD23 | 1:M:47:LEU:O    | 2.19                     | 0.43              |
| 1:S:47:LEU:HD23 | 1:S:47:LEU:O    | 2.18                     | 0.43              |
| 1:V:47:LEU:HD23 | 1:V:47:LEU:O    | 2.19                     | 0.43              |
| 1:m:47:LEU:HD23 | 1:m:47:LEU:O    | 2.18                     | 0.43              |
| 1:w:196:PHE:HE1 | 1:y:86:LEU:HD11 | 1.82                     | 0.43              |
| 1:A:196:PHE:HE1 | 1:C:86:LEU:HD11 | 1.82                     | 0.43              |
| 1:C:47:LEU:HD23 | 1:C:47:LEU:O    | 2.19                     | 0.43              |
| 1:c:196:PHE:HE1 | 1:e:86:LEU:HD11 | 1.82                     | 0.43              |
| 1:e:47:LEU:HD23 | 1:e:47:LEU:O    | 2.19                     | 0.43              |
| 1:g:47:LEU:HD23 | 1:g:47:LEU:O    | 2.19                     | 0.43              |
| 1:j:47:LEU:HD23 | 1:j:47:LEU:O    | 2.19                     | 0.43              |
| 1:l:47:LEU:HD23 | 1:l:47:LEU:O    | 2.19                     | 0.43              |
| 1:r:47:LEU:HD23 | 1:r:47:LEU:O    | 2.18                     | 0.43              |
| 1:s:47:LEU:HD23 | 1:s:47:LEU:O    | 2.18                     | 0.43              |
| 1:y:47:LEU:HD23 | 1:y:47:LEU:O    | 2.19                     | 0.43              |
| 1:4:196:PHE:HE1 | 1:6:86:LEU:HD11 | 1.82                     | 0.43              |
| 1:U:47:LEU:HD23 | 1:U:47:LEU:O    | 2.19                     | 0.43              |
| 1:k:96:SER:O    | 1:k:99:SER:OG   | 2.30                     | 0.43              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:t:47:LEU:HD23 | 1:t:47:LEU:O    | 2.18                     | 0.43              |
| 1:u:47:LEU:HD23 | 1:u:47:LEU:O    | 2.18                     | 0.43              |
| 1:v:47:LEU:HD23 | 1:v:47:LEU:O    | 2.19                     | 0.43              |
| 1:H:47:LEU:HD23 | 1:H:47:LEU:O    | 2.18                     | 0.43              |
| 1:W:47:LEU:HD23 | 1:W:47:LEU:O    | 2.18                     | 0.43              |
| 1:a:47:LEU:HD23 | 1:a:47:LEU:O    | 2.18                     | 0.43              |
| 1:b:47:LEU:HD23 | 1:b:47:LEU:O    | 2.18                     | 0.43              |
| 1:2:47:LEU:HD23 | 1:2:47:LEU:O    | 2.18                     | 0.43              |
| 1:3:47:LEU:HD23 | 1:3:47:LEU:O    | 2.19                     | 0.43              |
| 1:Q:47:LEU:HD23 | 1:Q:47:LEU:O    | 2.19                     | 0.43              |
| 1:c:47:LEU:HD23 | 1:c:47:LEU:O    | 2.18                     | 0.43              |
| 1:i:47:LEU:HD23 | 1:i:47:LEU:O    | 2.19                     | 0.43              |
| 1:k:47:LEU:HD23 | 1:k:47:LEU:O    | 2.18                     | 0.43              |
| 1:w:96:SER:O    | 1:w:99:SER:OG   | 2.30                     | 0.43              |
| 1:G:47:LEU:HD23 | 1:G:47:LEU:O    | 2.18                     | 0.43              |
| 1:O:47:LEU:HD23 | 1:O:47:LEU:O    | 2.18                     | 0.43              |
| 1:T:47:LEU:HD23 | 1:T:47:LEU:O    | 2.19                     | 0.43              |
| 1:2:96:SER:O    | 1:2:99:SER:OG   | 2.30                     | 0.43              |
| 1:4:47:LEU:HD23 | 1:4:47:LEU:O    | 2.19                     | 0.43              |
| 1:G:196:PHE:HE1 | 1:I:86:LEU:HD11 | 1.82                     | 0.43              |
| 1:P:47:LEU:HD23 | 1:P:47:LEU:O    | 2.18                     | 0.43              |
| 1:x:47:LEU:HD23 | 1:x:47:LEU:O    | 2.19                     | 0.43              |
| 1:B:47:LEU:HD23 | 1:B:47:LEU:O    | 2.19                     | 0.43              |
| 1:L:47:LEU:HD23 | 1:L:47:LEU:O    | 2.18                     | 0.43              |
| 1:q:47:LEU:HD23 | 1:q:47:LEU:O    | 2.18                     | 0.43              |
| 1:7:47:LEU:HD23 | 1:7:47:LEU:O    | 2.18                     | 0.43              |
| 1:D:47:LEU:HD23 | 1:D:47:LEU:O    | 2.18                     | 0.43              |
| 1:I:47:LEU:HD23 | 1:I:47:LEU:O    | 2.18                     | 0.43              |
| 1:K:47:LEU:HD23 | 1:K:47:LEU:O    | 2.19                     | 0.43              |
| 1:X:47:LEU:HD23 | 1:X:47:LEU:O    | 2.19                     | 0.43              |
| 1:a:96:SER:O    | 1:a:99:SER:OG   | 2.30                     | 0.43              |
| 1:w:47:LEU:HD23 | 1:w:47:LEU:O    | 2.18                     | 0.43              |
| 1:2:196:PHE:HE1 | 1:4:86:LEU:HD11 | 1.82                     | 0.42              |
| 1:G:96:SER:O    | 1:G:99:SER:OG   | 2.30                     | 0.42              |
| 1:V:96:SER:O    | 1:V:99:SER:OG   | 2.30                     | 0.42              |
| 1:Y:47:LEU:HD23 | 1:Y:47:LEU:O    | 2.19                     | 0.42              |
| 1:z:47:LEU:HD23 | 1:z:47:LEU:O    | 2.18                     | 0.42              |
| 1:6:47:LEU:HD23 | 1:6:47:LEU:O    | 2.19                     | 0.42              |
| 1:o:47:LEU:HD23 | 1:o:47:LEU:O    | 2.19                     | 0.42              |
| 1:A:47:LEU:HD23 | 1:A:47:LEU:O    | 2.18                     | 0.42              |
| 1:F:43:LEU:HD13 | 1:I:145:SER:HA  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:J:47:LEU:HD23  | 1:J:47:LEU:O    | 2.18                     | 0.42              |
| 1:f:47:LEU:HD23  | 1:f:47:LEU:O    | 2.19                     | 0.42              |
| 1:n:47:LEU:HD23  | 1:n:47:LEU:O    | 2.18                     | 0.42              |
| 1:h:47:LEU:HD23  | 1:h:47:LEU:O    | 2.18                     | 0.42              |
| 1:I:196:PHE:HE1  | 1:K:86:LEU:HD11 | 1.83                     | 0.42              |
| 1:5:147:ILE:HG23 | 1:5:148:ALA:N   | 2.35                     | 0.42              |
| 1:G:147:ILE:HG23 | 1:G:148:ALA:N   | 2.35                     | 0.42              |
| 1:S:96:SER:O     | 1:S:99:SER:OG   | 2.30                     | 0.42              |
| 1:i:96:SER:O     | 1:i:99:SER:OG   | 2.30                     | 0.42              |
| 1:p:47:LEU:HD23  | 1:p:47:LEU:O    | 2.19                     | 0.42              |
| 1:2:147:ILE:HG23 | 1:2:148:ALA:N   | 2.35                     | 0.42              |
| 1:5:47:LEU:HD23  | 1:5:47:LEU:O    | 2.19                     | 0.42              |
| 1:O:147:ILE:HG23 | 1:O:148:ALA:N   | 2.35                     | 0.42              |
| 1:R:47:LEU:HD23  | 1:R:47:LEU:O    | 2.18                     | 0.42              |
| 1:Z:47:LEU:HD23  | 1:Z:47:LEU:O    | 2.18                     | 0.42              |
| 1:q:147:ILE:HG23 | 1:q:148:ALA:N   | 2.35                     | 0.42              |
| 1:z:147:ILE:HG23 | 1:z:148:ALA:N   | 2.35                     | 0.42              |
| 1:D:147:ILE:HG23 | 1:D:148:ALA:N   | 2.35                     | 0.42              |
| 1:J:147:ILE:HG23 | 1:J:148:ALA:N   | 2.35                     | 0.42              |
| 1:R:147:ILE:HG23 | 1:R:148:ALA:N   | 2.35                     | 0.42              |
| 1:Y:96:SER:O     | 1:Y:99:SER:OG   | 2.30                     | 0.42              |
| 1:c:147:ILE:HG23 | 1:c:148:ALA:N   | 2.35                     | 0.42              |
| 1:t:147:ILE:HG23 | 1:t:148:ALA:N   | 2.35                     | 0.42              |
| 1:L:147:ILE:HG23 | 1:L:148:ALA:N   | 2.35                     | 0.42              |
| 1:Z:147:ILE:HG23 | 1:Z:148:ALA:N   | 2.35                     | 0.42              |
| 1:i:147:ILE:HG23 | 1:i:148:ALA:N   | 2.35                     | 0.42              |
| 1:k:147:ILE:HG23 | 1:k:148:ALA:N   | 2.35                     | 0.42              |
| 1:q:170:ARG:O    | 1:q:173:THR:OG1 | 2.36                     | 0.42              |
| 1:x:147:ILE:HG23 | 1:x:148:ALA:N   | 2.35                     | 0.42              |
| 1:q:96:SER:O     | 1:q:99:SER:OG   | 2.30                     | 0.42              |
| 1:7:147:ILE:HG23 | 1:7:148:ALA:N   | 2.35                     | 0.41              |
| 1:B:147:ILE:HG23 | 1:B:148:ALA:N   | 2.35                     | 0.41              |
| 1:U:147:ILE:HG23 | 1:U:148:ALA:N   | 2.35                     | 0.41              |
| 1:W:147:ILE:HG23 | 1:W:148:ALA:N   | 2.35                     | 0.41              |
| 1:M:147:ILE:HG23 | 1:M:148:ALA:N   | 2.35                     | 0.41              |
| 1:l:147:ILE:HG23 | 1:l:148:ALA:N   | 2.35                     | 0.41              |
| 1:s:147:ILE:HG23 | 1:s:148:ALA:N   | 2.35                     | 0.41              |
| 1:A:147:ILE:HG23 | 1:A:148:ALA:N   | 2.35                     | 0.41              |
| 1:J:170:ARG:O    | 1:J:173:THR:OG1 | 2.36                     | 0.41              |
| 1:a:147:ILE:HG23 | 1:a:148:ALA:N   | 2.35                     | 0.41              |
| 1:X:147:ILE:HG23 | 1:X:148:ALA:N   | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:170:ARG:O    | 1:X:173:THR:OG1  | 2.36                     | 0.41              |
| 1:h:147:ILE:HG23 | 1:h:148:ALA:N    | 2.35                     | 0.41              |
| 1:z:170:ARG:O    | 1:z:173:THR:OG1  | 2.36                     | 0.41              |
| 1:0:147:ILE:HG23 | 1:0:148:ALA:N    | 2.35                     | 0.41              |
| 1:7:170:ARG:O    | 1:7:173:THR:OG1  | 2.36                     | 0.41              |
| 1:f:147:ILE:HG23 | 1:f:148:ALA:N    | 2.35                     | 0.41              |
| 1:j:147:ILE:HG23 | 1:j:148:ALA:N    | 2.35                     | 0.41              |
| 1:o:147:ILE:HG23 | 1:o:148:ALA:N    | 2.35                     | 0.41              |
| 1:D:170:ARG:O    | 1:D:173:THR:OG1  | 2.36                     | 0.41              |
| 1:E:147:ILE:HG23 | 1:E:148:ALA:N    | 2.35                     | 0.41              |
| 1:P:147:ILE:HG23 | 1:P:148:ALA:N    | 2.35                     | 0.41              |
| 1:T:147:ILE:HG23 | 1:T:148:ALA:N    | 2.35                     | 0.41              |
| 1:e:147:ILE:HG23 | 1:e:148:ALA:N    | 2.35                     | 0.41              |
| 1:l:170:ARG:O    | 1:l:173:THR:OG1  | 2.36                     | 0.41              |
| 1:I:147:ILE:HG23 | 1:I:148:ALA:N    | 2.35                     | 0.41              |
| 1:P:96:SER:O     | 1:P:99:SER:OG    | 2.30                     | 0.41              |
| 1:Y:147:ILE:HG23 | 1:Y:148:ALA:N    | 2.35                     | 0.41              |
| 1:b:147:ILE:HG23 | 1:b:148:ALA:N    | 2.35                     | 0.41              |
| 1:n:147:ILE:HG23 | 1:n:148:ALA:N    | 2.35                     | 0.41              |
| 1:w:147:ILE:HG23 | 1:w:148:ALA:N    | 2.35                     | 0.41              |
| 1:3:147:ILE:HG23 | 1:3:148:ALA:N    | 2.35                     | 0.41              |
| 1:4:147:ILE:HG23 | 1:4:148:ALA:N    | 2.35                     | 0.41              |
| 1:F:147:ILE:HG23 | 1:F:148:ALA:N    | 2.35                     | 0.41              |
| 1:H:147:ILE:HG23 | 1:H:148:ALA:N    | 2.35                     | 0.41              |
| 1:R:57:THR:CG2   | 1:R:108:LEU:HD11 | 2.51                     | 0.41              |
| 1:g:147:ILE:HG23 | 1:g:148:ALA:N    | 2.35                     | 0.41              |
| 1:m:147:ILE:HG23 | 1:m:148:ALA:N    | 2.35                     | 0.41              |
| 1:r:147:ILE:HG23 | 1:r:148:ALA:N    | 2.35                     | 0.41              |
| 1:v:147:ILE:HG23 | 1:v:148:ALA:N    | 2.35                     | 0.41              |
| 1:D:57:THR:CG2   | 1:D:108:LEU:HD11 | 2.51                     | 0.41              |
| 1:N:57:THR:CG2   | 1:N:108:LEU:HD11 | 2.51                     | 0.41              |
| 1:u:57:THR:CG2   | 1:u:108:LEU:HD11 | 2.51                     | 0.41              |
| 1:v:57:THR:CG2   | 1:v:108:LEU:HD11 | 2.51                     | 0.41              |
| 1:z:57:THR:CG2   | 1:z:108:LEU:HD11 | 2.51                     | 0.41              |
| 1:1:147:ILE:HG23 | 1:1:148:ALA:N    | 2.35                     | 0.40              |
| 1:S:147:ILE:HG23 | 1:S:148:ALA:N    | 2.35                     | 0.40              |
| 1:U:57:THR:CG2   | 1:U:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:V:57:THR:CG2   | 1:V:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:W:57:THR:CG2   | 1:W:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:b:57:THR:CG2   | 1:b:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:d:147:ILE:HG23 | 1:d:148:ALA:N    | 2.35                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:f:57:THR:CG2   | 1:f:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:k:57:THR:CG2   | 1:k:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:p:57:THR:CG2   | 1:p:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:r:57:THR:CG2   | 1:r:108:LEU:HD11 | 2.52                     | 0.40              |
| 1:u:147:ILE:HG23 | 1:u:148:ALA:N    | 2.35                     | 0.40              |
| 1:B:57:THR:CG2   | 1:B:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:Q:147:ILE:HG23 | 1:Q:148:ALA:N    | 2.35                     | 0.40              |
| 1:R:170:ARG:O    | 1:R:173:THR:OG1  | 2.36                     | 0.40              |
| 1:S:57:THR:CG2   | 1:S:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:X:57:THR:CG2   | 1:X:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:g:57:THR:CG2   | 1:g:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:l:57:THR:CG2   | 1:l:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:o:57:THR:CG2   | 1:o:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:q:57:THR:CG2   | 1:q:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:t:57:THR:CG2   | 1:t:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:4:57:THR:CG2   | 1:4:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:I:57:THR:CG2   | 1:I:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:P:57:THR:CG2   | 1:P:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:V:147:ILE:HG23 | 1:V:148:ALA:N    | 2.35                     | 0.40              |
| 1:Y:57:THR:CG2   | 1:Y:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:a:57:THR:CG2   | 1:a:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:b:96:SER:O     | 1:b:99:SER:OG    | 2.30                     | 0.40              |
| 1:c:57:THR:CG2   | 1:c:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:s:96:SER:O     | 1:s:99:SER:OG    | 2.30                     | 0.40              |
| 1:w:57:THR:CG2   | 1:w:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:x:57:THR:CG2   | 1:x:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:E:57:THR:CG2   | 1:E:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:I:43:LEU:HD13  | 1:L:145:SER:HA   | 2.04                     | 0.40              |
| 1:M:57:THR:CG2   | 1:M:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:O:57:THR:CG2   | 1:O:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:n:57:THR:CG2   | 1:n:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:p:147:ILE:HG23 | 1:p:148:ALA:N    | 2.35                     | 0.40              |
| 1:2:159:LEU:HD12 | 1:2:159:LEU:N    | 2.37                     | 0.40              |
| 1:6:57:THR:CG2   | 1:6:108:LEU:HD11 | 2.52                     | 0.40              |
| 1:7:159:LEU:HD12 | 1:7:159:LEU:N    | 2.37                     | 0.40              |
| 1:G:159:LEU:N    | 1:G:159:LEU:HD12 | 2.37                     | 0.40              |
| 1:K:57:THR:CG2   | 1:K:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:M:159:LEU:N    | 1:M:159:LEU:HD12 | 2.37                     | 0.40              |
| 1:N:147:ILE:HG23 | 1:N:148:ALA:N    | 2.35                     | 0.40              |
| 1:R:159:LEU:HD12 | 1:R:159:LEU:N    | 2.37                     | 0.40              |
| 1:W:159:LEU:HD12 | 1:W:159:LEU:N    | 2.37                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:b:159:LEU:N    | 1:b:159:LEU:HD12 | 2.37                     | 0.40              |
| 1:h:159:LEU:HD12 | 1:h:159:LEU:N    | 2.37                     | 0.40              |
| 1:i:57:THR:CG2   | 1:i:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:m:57:THR:CG2   | 1:m:108:LEU:HD11 | 2.51                     | 0.40              |
| 1:q:159:LEU:N    | 1:q:159:LEU:HD12 | 2.37                     | 0.40              |
| 1:y:147:ILE:HG23 | 1:y:148:ALA:N    | 2.35                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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   | 0     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | 1     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | 2     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | 3     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | 4     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | 5     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | 6     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | 7     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | A     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | B     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | C     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | D     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | E     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | F     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | G     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | H     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | I     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | J     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | K     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | L     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | M     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | N     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | O     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | P     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | Q     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | R     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | S     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | T     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | U     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | V     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | W     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | X     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | Y     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | Z     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | a     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | b     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | c     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | d     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | e     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | f     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | g     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | h     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | i     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | j     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | k     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 1   | l     | 194/246 (79%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured     | Allowed | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|---------|----------|-------------|-----|
| 1   | m     | 194/246 (79%)     | 193 (100%)   | 1 (0%)  | 0        | 100         | 100 |
| 1   | n     | 194/246 (79%)     | 193 (100%)   | 1 (0%)  | 0        | 100         | 100 |
| 1   | o     | 194/246 (79%)     | 193 (100%)   | 1 (0%)  | 0        | 100         | 100 |
| 1   | p     | 194/246 (79%)     | 193 (100%)   | 1 (0%)  | 0        | 100         | 100 |
| 1   | q     | 194/246 (79%)     | 193 (100%)   | 1 (0%)  | 0        | 100         | 100 |
| 1   | r     | 194/246 (79%)     | 193 (100%)   | 1 (0%)  | 0        | 100         | 100 |
| 1   | s     | 194/246 (79%)     | 193 (100%)   | 1 (0%)  | 0        | 100         | 100 |
| 1   | t     | 194/246 (79%)     | 193 (100%)   | 1 (0%)  | 0        | 100         | 100 |
| 1   | u     | 194/246 (79%)     | 193 (100%)   | 1 (0%)  | 0        | 100         | 100 |
| 1   | v     | 194/246 (79%)     | 193 (100%)   | 1 (0%)  | 0        | 100         | 100 |
| 1   | w     | 194/246 (79%)     | 193 (100%)   | 1 (0%)  | 0        | 100         | 100 |
| 1   | x     | 194/246 (79%)     | 193 (100%)   | 1 (0%)  | 0        | 100         | 100 |
| 1   | y     | 194/246 (79%)     | 193 (100%)   | 1 (0%)  | 0        | 100         | 100 |
| 1   | z     | 194/246 (79%)     | 193 (100%)   | 1 (0%)  | 0        | 100         | 100 |
| All | All   | 11640/14760 (79%) | 11580 (100%) | 60 (0%) | 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   | 0     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | 1     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | 2     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | 3     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | 4     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | 5     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | 6     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | 7     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | A     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | B     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | C     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | D     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | E     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | F     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | G     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | H     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | I     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | J     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | K     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | L     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | M     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | N     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | O     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | P     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | Q     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | R     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | S     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | T     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | U     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | V     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | W     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | X     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | Y     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | Z     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | a     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | b     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | c     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | d     | 163/208 (78%) | 163 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 1   | e     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | f     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | g     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | h     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | i     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | j     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | k     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | l     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | m     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | n     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | o     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | p     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | q     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | r     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | s     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | t     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | u     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | v     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | w     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | x     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | y     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| 1   | z     | 163/208 (78%)    | 163 (100%)  | 0        | 100         | 100 |
| All | All   | 9780/12480 (78%) | 9780 (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 (67) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 117 | GLN  |
| 1   | 1     | 117 | GLN  |
| 1   | 2     | 117 | GLN  |
| 1   | 3     | 117 | GLN  |
| 1   | 4     | 117 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 5     | 117 | GLN  |
| 1   | 6     | 117 | GLN  |
| 1   | 7     | 117 | GLN  |
| 1   | A     | 117 | GLN  |
| 1   | A     | 203 | GLN  |
| 1   | B     | 117 | GLN  |
| 1   | C     | 117 | GLN  |
| 1   | D     | 117 | GLN  |
| 1   | E     | 117 | GLN  |
| 1   | F     | 117 | GLN  |
| 1   | G     | 117 | GLN  |
| 1   | G     | 203 | GLN  |
| 1   | H     | 117 | GLN  |
| 1   | I     | 117 | GLN  |
| 1   | I     | 203 | GLN  |
| 1   | J     | 117 | GLN  |
| 1   | K     | 117 | GLN  |
| 1   | L     | 117 | GLN  |
| 1   | L     | 203 | GLN  |
| 1   | M     | 117 | GLN  |
| 1   | N     | 117 | GLN  |
| 1   | O     | 117 | GLN  |
| 1   | O     | 203 | GLN  |
| 1   | P     | 117 | GLN  |
| 1   | Q     | 117 | GLN  |
| 1   | R     | 117 | GLN  |
| 1   | R     | 203 | GLN  |
| 1   | S     | 117 | GLN  |
| 1   | T     | 117 | GLN  |
| 1   | U     | 117 | GLN  |
| 1   | V     | 117 | GLN  |
| 1   | W     | 117 | GLN  |
| 1   | X     | 117 | GLN  |
| 1   | Y     | 117 | GLN  |
| 1   | Z     | 117 | GLN  |
| 1   | a     | 117 | GLN  |
| 1   | b     | 117 | GLN  |
| 1   | c     | 117 | GLN  |
| 1   | d     | 117 | GLN  |
| 1   | e     | 117 | GLN  |
| 1   | f     | 117 | GLN  |
| 1   | g     | 117 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | h     | 117 | GLN  |
| 1   | i     | 117 | GLN  |
| 1   | j     | 117 | GLN  |
| 1   | k     | 117 | GLN  |
| 1   | l     | 117 | GLN  |
| 1   | l     | 203 | GLN  |
| 1   | m     | 117 | GLN  |
| 1   | n     | 117 | GLN  |
| 1   | o     | 117 | GLN  |
| 1   | p     | 117 | GLN  |
| 1   | q     | 117 | GLN  |
| 1   | r     | 117 | GLN  |
| 1   | s     | 117 | GLN  |
| 1   | t     | 117 | GLN  |
| 1   | u     | 117 | GLN  |
| 1   | v     | 117 | GLN  |
| 1   | w     | 117 | GLN  |
| 1   | x     | 117 | GLN  |
| 1   | y     | 117 | GLN  |
| 1   | z     | 117 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

60 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 |
| 2   | ADP  | w     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | i     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | Y     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | E     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | P     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | f     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | r     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | M     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | n     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | t     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | O     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | e     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | H     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | 3     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | U     | 301 | -    | 28,29,29     | 1.44 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | J     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | u     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | S     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | s     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | 2     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | z     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | 7     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | m     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | V     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | D     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | X     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | G     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | o     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | L     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | T     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | 5     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | B     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | ADP  | v     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | F     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | C     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | g     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | a     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | W     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | j     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | 4     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | q     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | d     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | y     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | I     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | Q     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | l     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | k     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | x     | 301 | -    | 28,29,29     | 1.44 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | b     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | l     | 301 | -    | 28,29,29     | 1.44 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | h     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | K     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | R     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | 0     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | Z     | 301 | -    | 28,29,29     | 1.43 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | c     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | 6     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | N     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |
| 2   | ADP  | p     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.90 | 10 (23%) |
| 2   | ADP  | A     | 301 | -    | 28,29,29     | 1.42 | 5 (17%)  | 43,45,45    | 1.89 | 10 (23%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | ADP  | w     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | ADP  | i     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | Y     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | E     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | P     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | f     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | r     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | M     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | n     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | t     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | O     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | e     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | H     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | 3     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | U     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | J     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | u     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | S     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | s     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | 2     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | z     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | 7     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | m     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | V     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | D     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | X     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | G     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | o     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | L     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | T     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | 5     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | B     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | v     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | F     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | C     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | ADP  | g     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | a     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | W     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | j     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | 4     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | q     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | d     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | y     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | I     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | Q     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | l     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | k     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | x     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | b     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | l     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | h     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | K     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | R     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | 0     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | Z     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | c     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | 6     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | N     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | p     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 2   | ADP  | A     | 301 | -    | -       | 8/16/32/32 | 0/3/3/3 |

All (300) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | U     | 301 | ADP  | C5-C4 | 4.64 | 1.47        | 1.39     |
| 2   | 7     | 301 | ADP  | C5-C4 | 4.64 | 1.47        | 1.39     |
| 2   | D     | 301 | ADP  | C5-C4 | 4.63 | 1.47        | 1.39     |
| 2   | z     | 301 | ADP  | C5-C4 | 4.63 | 1.47        | 1.39     |
| 2   | l     | 301 | ADP  | C5-C4 | 4.63 | 1.47        | 1.39     |
| 2   | a     | 301 | ADP  | C5-C4 | 4.63 | 1.47        | 1.39     |
| 2   | V     | 301 | ADP  | C5-C4 | 4.62 | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | v     | 301 | ADP  | C5-C4 | 4.62 | 1.47        | 1.39     |
| 2   | G     | 301 | ADP  | C5-C4 | 4.61 | 1.47        | 1.39     |
| 2   | 3     | 301 | ADP  | C5-C4 | 4.61 | 1.47        | 1.39     |
| 2   | X     | 301 | ADP  | C5-C4 | 4.61 | 1.47        | 1.39     |
| 2   | H     | 301 | ADP  | C5-C4 | 4.61 | 1.47        | 1.39     |
| 2   | W     | 301 | ADP  | C5-C4 | 4.61 | 1.47        | 1.39     |
| 2   | e     | 301 | ADP  | C5-C4 | 4.61 | 1.47        | 1.39     |
| 2   | E     | 301 | ADP  | C5-C4 | 4.61 | 1.47        | 1.39     |
| 2   | N     | 301 | ADP  | C5-C4 | 4.61 | 1.47        | 1.39     |
| 2   | Z     | 301 | ADP  | C5-C4 | 4.61 | 1.47        | 1.39     |
| 2   | 6     | 301 | ADP  | C5-C4 | 4.61 | 1.47        | 1.39     |
| 2   | K     | 301 | ADP  | C5-C4 | 4.60 | 1.47        | 1.39     |
| 2   | C     | 301 | ADP  | C5-C4 | 4.60 | 1.47        | 1.39     |
| 2   | x     | 301 | ADP  | C5-C4 | 4.60 | 1.47        | 1.39     |
| 2   | k     | 301 | ADP  | C5-C4 | 4.60 | 1.47        | 1.39     |
| 2   | j     | 301 | ADP  | C5-C4 | 4.60 | 1.47        | 1.39     |
| 2   | 4     | 301 | ADP  | C5-C4 | 4.60 | 1.47        | 1.39     |
| 2   | b     | 301 | ADP  | C5-C4 | 4.60 | 1.47        | 1.39     |
| 2   | I     | 301 | ADP  | C5-C4 | 4.60 | 1.47        | 1.39     |
| 2   | f     | 301 | ADP  | C5-C4 | 4.60 | 1.47        | 1.39     |
| 2   | 0     | 301 | ADP  | C5-C4 | 4.59 | 1.47        | 1.39     |
| 2   | Q     | 301 | ADP  | C5-C4 | 4.59 | 1.47        | 1.39     |
| 2   | F     | 301 | ADP  | C5-C4 | 4.59 | 1.47        | 1.39     |
| 2   | r     | 301 | ADP  | C5-C4 | 4.59 | 1.47        | 1.39     |
| 2   | d     | 301 | ADP  | C5-C4 | 4.59 | 1.47        | 1.39     |
| 2   | i     | 301 | ADP  | C5-C4 | 4.59 | 1.47        | 1.39     |
| 2   | L     | 301 | ADP  | C5-C4 | 4.58 | 1.47        | 1.39     |
| 2   | M     | 301 | ADP  | C5-C4 | 4.58 | 1.47        | 1.39     |
| 2   | h     | 301 | ADP  | C5-C4 | 4.58 | 1.47        | 1.39     |
| 2   | m     | 301 | ADP  | C5-C4 | 4.58 | 1.47        | 1.39     |
| 2   | c     | 301 | ADP  | C5-C4 | 4.58 | 1.47        | 1.39     |
| 2   | 5     | 301 | ADP  | C5-C4 | 4.58 | 1.47        | 1.39     |
| 2   | R     | 301 | ADP  | C5-C4 | 4.58 | 1.47        | 1.39     |
| 2   | Y     | 301 | ADP  | C5-C4 | 4.58 | 1.47        | 1.39     |
| 2   | 2     | 301 | ADP  | C5-C4 | 4.58 | 1.47        | 1.39     |
| 2   | g     | 301 | ADP  | C5-C4 | 4.58 | 1.47        | 1.39     |
| 2   | A     | 301 | ADP  | C5-C4 | 4.57 | 1.47        | 1.39     |
| 2   | n     | 301 | ADP  | C5-C4 | 4.57 | 1.47        | 1.39     |
| 2   | S     | 301 | ADP  | C5-C4 | 4.57 | 1.47        | 1.39     |
| 2   | P     | 301 | ADP  | C5-C4 | 4.57 | 1.47        | 1.39     |
| 2   | B     | 301 | ADP  | C5-C4 | 4.57 | 1.47        | 1.39     |
| 2   | u     | 301 | ADP  | C5-C4 | 4.57 | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | w     | 301 | ADP  | C5-C4 | 4.57 | 1.47        | 1.39     |
| 2   | p     | 301 | ADP  | C5-C4 | 4.57 | 1.47        | 1.39     |
| 2   | s     | 301 | ADP  | C5-C4 | 4.57 | 1.47        | 1.39     |
| 2   | T     | 301 | ADP  | C5-C4 | 4.57 | 1.47        | 1.39     |
| 2   | l     | 301 | ADP  | C5-C4 | 4.56 | 1.47        | 1.39     |
| 2   | O     | 301 | ADP  | C5-C4 | 4.56 | 1.47        | 1.39     |
| 2   | y     | 301 | ADP  | C5-C4 | 4.56 | 1.47        | 1.39     |
| 2   | o     | 301 | ADP  | C5-C4 | 4.56 | 1.47        | 1.39     |
| 2   | J     | 301 | ADP  | C5-C4 | 4.56 | 1.47        | 1.39     |
| 2   | t     | 301 | ADP  | C5-C4 | 4.56 | 1.47        | 1.39     |
| 2   | q     | 301 | ADP  | C5-C4 | 4.55 | 1.47        | 1.39     |
| 2   | T     | 301 | ADP  | C5-C6 | 2.75 | 1.48        | 1.41     |
| 2   | C     | 301 | ADP  | C5-C6 | 2.75 | 1.48        | 1.41     |
| 2   | y     | 301 | ADP  | C5-C6 | 2.74 | 1.48        | 1.41     |
| 2   | m     | 301 | ADP  | C5-C6 | 2.74 | 1.48        | 1.41     |
| 2   | O     | 301 | ADP  | C5-C6 | 2.74 | 1.48        | 1.41     |
| 2   | G     | 301 | ADP  | C5-C6 | 2.74 | 1.48        | 1.41     |
| 2   | x     | 301 | ADP  | C5-C6 | 2.74 | 1.48        | 1.41     |
| 2   | f     | 301 | ADP  | C5-C6 | 2.74 | 1.48        | 1.41     |
| 2   | L     | 301 | ADP  | C5-C6 | 2.73 | 1.48        | 1.41     |
| 2   | d     | 301 | ADP  | C5-C6 | 2.73 | 1.48        | 1.41     |
| 2   | h     | 301 | ADP  | C5-C6 | 2.73 | 1.48        | 1.41     |
| 2   | W     | 301 | ADP  | C5-C6 | 2.73 | 1.48        | 1.41     |
| 2   | I     | 301 | ADP  | C5-C6 | 2.73 | 1.48        | 1.41     |
| 2   | w     | 301 | ADP  | C5-C6 | 2.72 | 1.48        | 1.41     |
| 2   | i     | 301 | ADP  | C5-C6 | 2.72 | 1.48        | 1.41     |
| 2   | o     | 301 | ADP  | C5-C6 | 2.72 | 1.48        | 1.41     |
| 2   | b     | 301 | ADP  | C5-C6 | 2.72 | 1.48        | 1.41     |
| 2   | Z     | 301 | ADP  | C5-C6 | 2.72 | 1.48        | 1.41     |
| 2   | j     | 301 | ADP  | C5-C6 | 2.72 | 1.48        | 1.41     |
| 2   | c     | 301 | ADP  | C5-C6 | 2.72 | 1.48        | 1.41     |
| 2   | J     | 301 | ADP  | C5-C6 | 2.72 | 1.48        | 1.41     |
| 2   | q     | 301 | ADP  | C5-C6 | 2.72 | 1.48        | 1.41     |
| 2   | 3     | 301 | ADP  | C5-C6 | 2.72 | 1.48        | 1.41     |
| 2   | M     | 301 | ADP  | C5-C6 | 2.72 | 1.48        | 1.41     |
| 2   | Y     | 301 | ADP  | C5-C6 | 2.72 | 1.48        | 1.41     |
| 2   | s     | 301 | ADP  | C5-C6 | 2.72 | 1.48        | 1.41     |
| 2   | D     | 301 | ADP  | C5-C6 | 2.71 | 1.48        | 1.41     |
| 2   | Q     | 301 | ADP  | C5-C6 | 2.71 | 1.48        | 1.41     |
| 2   | R     | 301 | ADP  | C5-C6 | 2.71 | 1.48        | 1.41     |
| 2   | l     | 301 | ADP  | C5-C6 | 2.71 | 1.48        | 1.41     |
| 2   | F     | 301 | ADP  | C5-C6 | 2.71 | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | H     | 301 | ADP  | C5-C6 | 2.71 | 1.48        | 1.41     |
| 2   | n     | 301 | ADP  | C5-C6 | 2.71 | 1.48        | 1.41     |
| 2   | z     | 301 | ADP  | C5-C6 | 2.71 | 1.48        | 1.41     |
| 2   | K     | 301 | ADP  | C5-C6 | 2.71 | 1.48        | 1.41     |
| 2   | X     | 301 | ADP  | C5-C6 | 2.71 | 1.48        | 1.41     |
| 2   | t     | 301 | ADP  | C5-C6 | 2.71 | 1.48        | 1.41     |
| 2   | 0     | 301 | ADP  | C5-C6 | 2.71 | 1.48        | 1.41     |
| 2   | V     | 301 | ADP  | C5-C6 | 2.71 | 1.48        | 1.41     |
| 2   | 4     | 301 | ADP  | C5-C6 | 2.71 | 1.48        | 1.41     |
| 2   | N     | 301 | ADP  | C5-C6 | 2.71 | 1.48        | 1.41     |
| 2   | U     | 301 | ADP  | C5-C6 | 2.71 | 1.48        | 1.41     |
| 2   | k     | 301 | ADP  | C5-C6 | 2.71 | 1.48        | 1.41     |
| 2   | 5     | 301 | ADP  | C5-C6 | 2.71 | 1.48        | 1.41     |
| 2   | g     | 301 | ADP  | C5-C6 | 2.70 | 1.48        | 1.41     |
| 2   | B     | 301 | ADP  | C5-C6 | 2.70 | 1.48        | 1.41     |
| 2   | 6     | 301 | ADP  | C5-C6 | 2.70 | 1.48        | 1.41     |
| 2   | 7     | 301 | ADP  | C5-C6 | 2.70 | 1.48        | 1.41     |
| 2   | p     | 301 | ADP  | C5-C6 | 2.70 | 1.48        | 1.41     |
| 2   | u     | 301 | ADP  | C5-C6 | 2.70 | 1.48        | 1.41     |
| 2   | A     | 301 | ADP  | C5-C6 | 2.70 | 1.48        | 1.41     |
| 2   | E     | 301 | ADP  | C5-C6 | 2.70 | 1.48        | 1.41     |
| 2   | e     | 301 | ADP  | C5-C6 | 2.70 | 1.48        | 1.41     |
| 2   | v     | 301 | ADP  | C5-C6 | 2.70 | 1.48        | 1.41     |
| 2   | S     | 301 | ADP  | C5-C6 | 2.69 | 1.48        | 1.41     |
| 2   | 2     | 301 | ADP  | C5-C6 | 2.69 | 1.48        | 1.41     |
| 2   | P     | 301 | ADP  | C5-C6 | 2.69 | 1.48        | 1.41     |
| 2   | a     | 301 | ADP  | C5-C6 | 2.68 | 1.48        | 1.41     |
| 2   | r     | 301 | ADP  | C5-C6 | 2.68 | 1.48        | 1.41     |
| 2   | l     | 301 | ADP  | C5-C6 | 2.68 | 1.48        | 1.41     |
| 2   | l     | 301 | ADP  | C8-N7 | 2.46 | 1.36        | 1.31     |
| 2   | 3     | 301 | ADP  | C8-N7 | 2.45 | 1.36        | 1.31     |
| 2   | L     | 301 | ADP  | C8-N7 | 2.45 | 1.36        | 1.31     |
| 2   | E     | 301 | ADP  | C8-N7 | 2.45 | 1.36        | 1.31     |
| 2   | F     | 301 | ADP  | C8-N7 | 2.45 | 1.36        | 1.31     |
| 2   | H     | 301 | ADP  | C8-N7 | 2.44 | 1.36        | 1.31     |
| 2   | S     | 301 | ADP  | C8-N7 | 2.44 | 1.36        | 1.31     |
| 2   | R     | 301 | ADP  | C8-N7 | 2.44 | 1.36        | 1.31     |
| 2   | o     | 301 | ADP  | C8-N7 | 2.44 | 1.36        | 1.31     |
| 2   | A     | 301 | ADP  | C8-N7 | 2.44 | 1.36        | 1.31     |
| 2   | T     | 301 | ADP  | C8-N7 | 2.44 | 1.36        | 1.31     |
| 2   | u     | 301 | ADP  | C8-N7 | 2.44 | 1.36        | 1.31     |
| 2   | U     | 301 | ADP  | C8-N7 | 2.43 | 1.36        | 1.31     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | 1     | 301 | ADP  | C8-N7 | 2.43 | 1.36        | 1.31     |
| 2   | C     | 301 | ADP  | C8-N7 | 2.43 | 1.36        | 1.31     |
| 2   | d     | 301 | ADP  | C8-N7 | 2.43 | 1.36        | 1.31     |
| 2   | w     | 301 | ADP  | C8-N7 | 2.43 | 1.36        | 1.31     |
| 2   | X     | 301 | ADP  | C8-N7 | 2.43 | 1.36        | 1.31     |
| 2   | t     | 301 | ADP  | C8-N7 | 2.42 | 1.36        | 1.31     |
| 2   | x     | 301 | ADP  | C8-N7 | 2.42 | 1.36        | 1.31     |
| 2   | j     | 301 | ADP  | C8-N7 | 2.42 | 1.36        | 1.31     |
| 2   | B     | 301 | ADP  | C8-N7 | 2.42 | 1.36        | 1.31     |
| 2   | i     | 301 | ADP  | C8-N7 | 2.42 | 1.36        | 1.31     |
| 2   | b     | 301 | ADP  | C8-N7 | 2.42 | 1.36        | 1.31     |
| 2   | 7     | 301 | ADP  | C8-N7 | 2.42 | 1.36        | 1.31     |
| 2   | p     | 301 | ADP  | C8-N7 | 2.42 | 1.36        | 1.31     |
| 2   | f     | 301 | ADP  | C8-N7 | 2.42 | 1.36        | 1.31     |
| 2   | r     | 301 | ADP  | C8-N7 | 2.42 | 1.36        | 1.31     |
| 2   | W     | 301 | ADP  | C8-N7 | 2.42 | 1.36        | 1.31     |
| 2   | D     | 301 | ADP  | C8-N7 | 2.42 | 1.36        | 1.31     |
| 2   | c     | 301 | ADP  | C8-N7 | 2.42 | 1.36        | 1.31     |
| 2   | k     | 301 | ADP  | C8-N7 | 2.41 | 1.36        | 1.31     |
| 2   | q     | 301 | ADP  | C8-N7 | 2.41 | 1.36        | 1.31     |
| 2   | 2     | 301 | ADP  | C8-N7 | 2.41 | 1.36        | 1.31     |
| 2   | n     | 301 | ADP  | C8-N7 | 2.41 | 1.36        | 1.31     |
| 2   | 0     | 301 | ADP  | C8-N7 | 2.41 | 1.36        | 1.31     |
| 2   | J     | 301 | ADP  | C8-N7 | 2.41 | 1.36        | 1.31     |
| 2   | 5     | 301 | ADP  | C8-N7 | 2.41 | 1.36        | 1.31     |
| 2   | a     | 301 | ADP  | C8-N7 | 2.41 | 1.36        | 1.31     |
| 2   | 4     | 301 | ADP  | C8-N7 | 2.40 | 1.36        | 1.31     |
| 2   | O     | 301 | ADP  | C8-N7 | 2.40 | 1.36        | 1.31     |
| 2   | Z     | 301 | ADP  | C8-N7 | 2.40 | 1.36        | 1.31     |
| 2   | M     | 301 | ADP  | C8-N7 | 2.40 | 1.36        | 1.31     |
| 2   | Q     | 301 | ADP  | C8-N7 | 2.40 | 1.36        | 1.31     |
| 2   | K     | 301 | ADP  | C8-N7 | 2.40 | 1.36        | 1.31     |
| 2   | v     | 301 | ADP  | C8-N7 | 2.40 | 1.36        | 1.31     |
| 2   | m     | 301 | ADP  | C8-N7 | 2.40 | 1.36        | 1.31     |
| 2   | z     | 301 | ADP  | C8-N7 | 2.40 | 1.36        | 1.31     |
| 2   | h     | 301 | ADP  | C8-N7 | 2.40 | 1.36        | 1.31     |
| 2   | I     | 301 | ADP  | C8-N7 | 2.39 | 1.36        | 1.31     |
| 2   | s     | 301 | ADP  | C8-N7 | 2.39 | 1.36        | 1.31     |
| 2   | g     | 301 | ADP  | C8-N7 | 2.39 | 1.36        | 1.31     |
| 2   | e     | 301 | ADP  | C8-N7 | 2.39 | 1.36        | 1.31     |
| 2   | V     | 301 | ADP  | C8-N7 | 2.38 | 1.36        | 1.31     |
| 2   | G     | 301 | ADP  | C8-N7 | 2.38 | 1.36        | 1.31     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | N     | 301 | ADP  | C8-N7 | 2.37  | 1.36        | 1.31     |
| 2   | P     | 301 | ADP  | C8-N7 | 2.37  | 1.36        | 1.31     |
| 2   | y     | 301 | ADP  | C8-N7 | 2.37  | 1.36        | 1.31     |
| 2   | Y     | 301 | ADP  | C8-N7 | 2.37  | 1.36        | 1.31     |
| 2   | 6     | 301 | ADP  | C8-N7 | 2.35  | 1.36        | 1.31     |
| 2   | E     | 301 | ADP  | C5-N7 | -2.34 | 1.34        | 1.39     |
| 2   | O     | 301 | ADP  | C5-N7 | -2.34 | 1.34        | 1.39     |
| 2   | G     | 301 | ADP  | C5-N7 | -2.33 | 1.34        | 1.39     |
| 2   | y     | 301 | ADP  | C5-N7 | -2.33 | 1.34        | 1.39     |
| 2   | a     | 301 | ADP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 2   | N     | 301 | ADP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 2   | j     | 301 | ADP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 2   | m     | 301 | ADP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 2   | f     | 301 | ADP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 2   | J     | 301 | ADP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 2   | K     | 301 | ADP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 2   | S     | 301 | ADP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 2   | I     | 301 | ADP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 2   | c     | 301 | ADP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 2   | i     | 301 | ADP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 2   | x     | 301 | ADP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 2   | z     | 301 | ADP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 2   | T     | 301 | ADP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 2   | b     | 301 | ADP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 2   | s     | 301 | ADP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 2   | o     | 301 | ADP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 2   | L     | 301 | ADP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 2   | w     | 301 | ADP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 2   | D     | 301 | ADP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 2   | g     | 301 | ADP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 2   | r     | 301 | ADP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 2   | 7     | 301 | ADP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 2   | l     | 301 | ADP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 2   | h     | 301 | ADP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 2   | U     | 301 | ADP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 2   | C     | 301 | ADP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 2   | n     | 301 | ADP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 2   | V     | 301 | ADP  | C5-N7 | -2.29 | 1.34        | 1.39     |
| 2   | k     | 301 | ADP  | C5-N7 | -2.29 | 1.34        | 1.39     |
| 2   | u     | 301 | ADP  | C5-N7 | -2.29 | 1.34        | 1.39     |
| 2   | M     | 301 | ADP  | C5-N7 | -2.29 | 1.34        | 1.39     |
| 2   | 3     | 301 | ADP  | C5-N7 | -2.29 | 1.34        | 1.39     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | d     | 301 | ADP  | C5-N7  | -2.29 | 1.34        | 1.39     |
| 2   | p     | 301 | ADP  | C5-N7  | -2.29 | 1.34        | 1.39     |
| 2   | Q     | 301 | ADP  | C5-N7  | -2.29 | 1.34        | 1.39     |
| 2   | H     | 301 | ADP  | C5-N7  | -2.29 | 1.34        | 1.39     |
| 2   | e     | 301 | ADP  | C5-N7  | -2.28 | 1.34        | 1.39     |
| 2   | X     | 301 | ADP  | C5-N7  | -2.28 | 1.34        | 1.39     |
| 2   | W     | 301 | ADP  | C5-N7  | -2.28 | 1.34        | 1.39     |
| 2   | Z     | 301 | ADP  | C5-N7  | -2.28 | 1.34        | 1.39     |
| 2   | 4     | 301 | ADP  | C5-N7  | -2.28 | 1.34        | 1.39     |
| 2   | 5     | 301 | ADP  | C5-N7  | -2.28 | 1.34        | 1.39     |
| 2   | 0     | 301 | ADP  | C5-N7  | -2.28 | 1.34        | 1.39     |
| 2   | 2     | 301 | ADP  | C5-N7  | -2.28 | 1.34        | 1.39     |
| 2   | F     | 301 | ADP  | C5-N7  | -2.27 | 1.34        | 1.39     |
| 2   | t     | 301 | ADP  | C5-N7  | -2.27 | 1.34        | 1.39     |
| 2   | 6     | 301 | ADP  | C5-N7  | -2.27 | 1.34        | 1.39     |
| 2   | 1     | 301 | ADP  | C5-N7  | -2.27 | 1.34        | 1.39     |
| 2   | Y     | 301 | ADP  | C5-N7  | -2.27 | 1.34        | 1.39     |
| 2   | B     | 301 | ADP  | C5-N7  | -2.27 | 1.34        | 1.39     |
| 2   | q     | 301 | ADP  | C5-N7  | -2.27 | 1.34        | 1.39     |
| 2   | A     | 301 | ADP  | C5-N7  | -2.27 | 1.34        | 1.39     |
| 2   | v     | 301 | ADP  | C5-N7  | -2.26 | 1.35        | 1.39     |
| 2   | R     | 301 | ADP  | C5-N7  | -2.26 | 1.35        | 1.39     |
| 2   | P     | 301 | ADP  | C5-N7  | -2.26 | 1.35        | 1.39     |
| 2   | B     | 301 | ADP  | PA-O3A | 2.21  | 1.61        | 1.59     |
| 2   | f     | 301 | ADP  | PA-O3A | 2.19  | 1.61        | 1.59     |
| 2   | E     | 301 | ADP  | PA-O3A | 2.19  | 1.61        | 1.59     |
| 2   | G     | 301 | ADP  | PA-O3A | 2.19  | 1.61        | 1.59     |
| 2   | 5     | 301 | ADP  | PA-O3A | 2.19  | 1.61        | 1.59     |
| 2   | d     | 301 | ADP  | PA-O3A | 2.19  | 1.61        | 1.59     |
| 2   | o     | 301 | ADP  | PA-O3A | 2.19  | 1.61        | 1.59     |
| 2   | l     | 301 | ADP  | PA-O3A | 2.19  | 1.61        | 1.59     |
| 2   | 0     | 301 | ADP  | PA-O3A | 2.18  | 1.61        | 1.59     |
| 2   | a     | 301 | ADP  | PA-O3A | 2.18  | 1.61        | 1.59     |
| 2   | x     | 301 | ADP  | PA-O3A | 2.18  | 1.61        | 1.59     |
| 2   | J     | 301 | ADP  | PA-O3A | 2.18  | 1.61        | 1.59     |
| 2   | R     | 301 | ADP  | PA-O3A | 2.18  | 1.61        | 1.59     |
| 2   | t     | 301 | ADP  | PA-O3A | 2.17  | 1.61        | 1.59     |
| 2   | q     | 301 | ADP  | PA-O3A | 2.17  | 1.61        | 1.59     |
| 2   | S     | 301 | ADP  | PA-O3A | 2.17  | 1.61        | 1.59     |
| 2   | 2     | 301 | ADP  | PA-O3A | 2.17  | 1.61        | 1.59     |
| 2   | I     | 301 | ADP  | PA-O3A | 2.17  | 1.61        | 1.59     |
| 2   | U     | 301 | ADP  | PA-O3A | 2.17  | 1.61        | 1.59     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | P     | 301 | ADP  | PA-O3A | 2.17 | 1.61        | 1.59     |
| 2   | i     | 301 | ADP  | PA-O3A | 2.16 | 1.61        | 1.59     |
| 2   | M     | 301 | ADP  | PA-O3A | 2.15 | 1.61        | 1.59     |
| 2   | X     | 301 | ADP  | PA-O3A | 2.15 | 1.61        | 1.59     |
| 2   | e     | 301 | ADP  | PA-O3A | 2.14 | 1.61        | 1.59     |
| 2   | F     | 301 | ADP  | PA-O3A | 2.14 | 1.61        | 1.59     |
| 2   | l     | 301 | ADP  | PA-O3A | 2.13 | 1.61        | 1.59     |
| 2   | Z     | 301 | ADP  | PA-O3A | 2.13 | 1.61        | 1.59     |
| 2   | D     | 301 | ADP  | PA-O3A | 2.12 | 1.61        | 1.59     |
| 2   | T     | 301 | ADP  | PA-O3A | 2.12 | 1.61        | 1.59     |
| 2   | O     | 301 | ADP  | PA-O3A | 2.12 | 1.61        | 1.59     |
| 2   | g     | 301 | ADP  | PA-O3A | 2.12 | 1.61        | 1.59     |
| 2   | c     | 301 | ADP  | PA-O3A | 2.11 | 1.61        | 1.59     |
| 2   | W     | 301 | ADP  | PA-O3A | 2.11 | 1.61        | 1.59     |
| 2   | 3     | 301 | ADP  | PA-O3A | 2.11 | 1.61        | 1.59     |
| 2   | m     | 301 | ADP  | PA-O3A | 2.11 | 1.61        | 1.59     |
| 2   | u     | 301 | ADP  | PA-O3A | 2.11 | 1.61        | 1.59     |
| 2   | w     | 301 | ADP  | PA-O3A | 2.11 | 1.61        | 1.59     |
| 2   | K     | 301 | ADP  | PA-O3A | 2.11 | 1.61        | 1.59     |
| 2   | 6     | 301 | ADP  | PA-O3A | 2.10 | 1.61        | 1.59     |
| 2   | Q     | 301 | ADP  | PA-O3A | 2.10 | 1.61        | 1.59     |
| 2   | V     | 301 | ADP  | PA-O3A | 2.10 | 1.61        | 1.59     |
| 2   | z     | 301 | ADP  | PA-O3A | 2.10 | 1.61        | 1.59     |
| 2   | s     | 301 | ADP  | PA-O3A | 2.10 | 1.61        | 1.59     |
| 2   | 7     | 301 | ADP  | PA-O3A | 2.10 | 1.61        | 1.59     |
| 2   | p     | 301 | ADP  | PA-O3A | 2.10 | 1.61        | 1.59     |
| 2   | A     | 301 | ADP  | PA-O3A | 2.10 | 1.61        | 1.59     |
| 2   | N     | 301 | ADP  | PA-O3A | 2.09 | 1.61        | 1.59     |
| 2   | 4     | 301 | ADP  | PA-O3A | 2.09 | 1.61        | 1.59     |
| 2   | r     | 301 | ADP  | PA-O3A | 2.09 | 1.61        | 1.59     |
| 2   | b     | 301 | ADP  | PA-O3A | 2.08 | 1.61        | 1.59     |
| 2   | j     | 301 | ADP  | PA-O3A | 2.08 | 1.61        | 1.59     |
| 2   | y     | 301 | ADP  | PA-O3A | 2.08 | 1.61        | 1.59     |
| 2   | v     | 301 | ADP  | PA-O3A | 2.08 | 1.61        | 1.59     |
| 2   | Y     | 301 | ADP  | PA-O3A | 2.08 | 1.61        | 1.59     |
| 2   | C     | 301 | ADP  | PA-O3A | 2.08 | 1.61        | 1.59     |
| 2   | H     | 301 | ADP  | PA-O3A | 2.08 | 1.61        | 1.59     |
| 2   | L     | 301 | ADP  | PA-O3A | 2.08 | 1.61        | 1.59     |
| 2   | n     | 301 | ADP  | PA-O3A | 2.08 | 1.61        | 1.59     |
| 2   | h     | 301 | ADP  | PA-O3A | 2.07 | 1.61        | 1.59     |
| 2   | k     | 301 | ADP  | PA-O3A | 2.07 | 1.61        | 1.59     |

All (600) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | H     | 301 | ADP  | C5-C4-N3 | -5.74 | 118.81      | 126.72   |
| 2   | d     | 301 | ADP  | C5-C4-N3 | -5.74 | 118.81      | 126.72   |
| 2   | 3     | 301 | ADP  | C5-C4-N3 | -5.74 | 118.81      | 126.72   |
| 2   | Q     | 301 | ADP  | C5-C4-N3 | -5.74 | 118.82      | 126.72   |
| 2   | x     | 301 | ADP  | C5-C4-N3 | -5.74 | 118.82      | 126.72   |
| 2   | n     | 301 | ADP  | C5-C4-N3 | -5.74 | 118.82      | 126.72   |
| 2   | 6     | 301 | ADP  | C5-C4-N3 | -5.74 | 118.82      | 126.72   |
| 2   | l     | 301 | ADP  | C5-C4-N3 | -5.74 | 118.82      | 126.72   |
| 2   | P     | 301 | ADP  | C5-C4-N3 | -5.73 | 118.82      | 126.72   |
| 2   | 5     | 301 | ADP  | C5-C4-N3 | -5.73 | 118.82      | 126.72   |
| 2   | U     | 301 | ADP  | C5-C4-N3 | -5.73 | 118.82      | 126.72   |
| 2   | r     | 301 | ADP  | C5-C4-N3 | -5.73 | 118.83      | 126.72   |
| 2   | b     | 301 | ADP  | C5-C4-N3 | -5.73 | 118.83      | 126.72   |
| 2   | p     | 301 | ADP  | C5-C4-N3 | -5.73 | 118.83      | 126.72   |
| 2   | e     | 301 | ADP  | C5-C4-N3 | -5.72 | 118.83      | 126.72   |
| 2   | I     | 301 | ADP  | C5-C4-N3 | -5.72 | 118.84      | 126.72   |
| 2   | K     | 301 | ADP  | C5-C4-N3 | -5.72 | 118.84      | 126.72   |
| 2   | Z     | 301 | ADP  | C5-C4-N3 | -5.72 | 118.84      | 126.72   |
| 2   | 0     | 301 | ADP  | C5-C4-N3 | -5.72 | 118.84      | 126.72   |
| 2   | a     | 301 | ADP  | C5-C4-N3 | -5.72 | 118.84      | 126.72   |
| 2   | M     | 301 | ADP  | C5-C4-N3 | -5.72 | 118.84      | 126.72   |
| 2   | X     | 301 | ADP  | C5-C4-N3 | -5.72 | 118.84      | 126.72   |
| 2   | V     | 301 | ADP  | C5-C4-N3 | -5.72 | 118.85      | 126.72   |
| 2   | q     | 301 | ADP  | C5-C4-N3 | -5.72 | 118.85      | 126.72   |
| 2   | t     | 301 | ADP  | C5-C4-N3 | -5.71 | 118.85      | 126.72   |
| 2   | 1     | 301 | ADP  | C5-C4-N3 | -5.71 | 118.85      | 126.72   |
| 2   | J     | 301 | ADP  | C5-C4-N3 | -5.71 | 118.85      | 126.72   |
| 2   | c     | 301 | ADP  | C5-C4-N3 | -5.71 | 118.85      | 126.72   |
| 2   | k     | 301 | ADP  | C5-C4-N3 | -5.71 | 118.85      | 126.72   |
| 2   | m     | 301 | ADP  | C5-C4-N3 | -5.71 | 118.85      | 126.72   |
| 2   | o     | 301 | ADP  | C5-C4-N3 | -5.71 | 118.85      | 126.72   |
| 2   | L     | 301 | ADP  | C5-C4-N3 | -5.71 | 118.85      | 126.72   |
| 2   | G     | 301 | ADP  | C5-C4-N3 | -5.71 | 118.86      | 126.72   |
| 2   | W     | 301 | ADP  | C5-C4-N3 | -5.71 | 118.86      | 126.72   |
| 2   | C     | 301 | ADP  | C5-C4-N3 | -5.71 | 118.86      | 126.72   |
| 2   | i     | 301 | ADP  | C5-C4-N3 | -5.71 | 118.86      | 126.72   |
| 2   | 2     | 301 | ADP  | C5-C4-N3 | -5.71 | 118.86      | 126.72   |
| 2   | R     | 301 | ADP  | C5-C4-N3 | -5.71 | 118.86      | 126.72   |
| 2   | 7     | 301 | ADP  | C5-C4-N3 | -5.70 | 118.86      | 126.72   |
| 2   | v     | 301 | ADP  | C5-C4-N3 | -5.70 | 118.86      | 126.72   |
| 2   | S     | 301 | ADP  | C5-C4-N3 | -5.70 | 118.87      | 126.72   |
| 2   | 4     | 301 | ADP  | C5-C4-N3 | -5.70 | 118.87      | 126.72   |
| 2   | h     | 301 | ADP  | C5-C4-N3 | -5.70 | 118.87      | 126.72   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | D     | 301 | ADP  | C5-C4-N3 | -5.70 | 118.87      | 126.72   |
| 2   | B     | 301 | ADP  | C5-C4-N3 | -5.70 | 118.87      | 126.72   |
| 2   | g     | 301 | ADP  | C5-C4-N3 | -5.70 | 118.87      | 126.72   |
| 2   | y     | 301 | ADP  | C5-C4-N3 | -5.70 | 118.87      | 126.72   |
| 2   | s     | 301 | ADP  | C5-C4-N3 | -5.70 | 118.88      | 126.72   |
| 2   | w     | 301 | ADP  | C5-C4-N3 | -5.69 | 118.88      | 126.72   |
| 2   | T     | 301 | ADP  | C5-C4-N3 | -5.69 | 118.88      | 126.72   |
| 2   | f     | 301 | ADP  | C5-C4-N3 | -5.69 | 118.88      | 126.72   |
| 2   | z     | 301 | ADP  | C5-C4-N3 | -5.69 | 118.88      | 126.72   |
| 2   | u     | 301 | ADP  | C5-C4-N3 | -5.68 | 118.89      | 126.72   |
| 2   | A     | 301 | ADP  | C5-C4-N3 | -5.68 | 118.89      | 126.72   |
| 2   | F     | 301 | ADP  | C5-C4-N3 | -5.68 | 118.90      | 126.72   |
| 2   | Y     | 301 | ADP  | C5-C4-N3 | -5.68 | 118.90      | 126.72   |
| 2   | E     | 301 | ADP  | C5-C4-N3 | -5.68 | 118.90      | 126.72   |
| 2   | j     | 301 | ADP  | C5-C4-N3 | -5.67 | 118.91      | 126.72   |
| 2   | O     | 301 | ADP  | C5-C4-N3 | -5.67 | 118.91      | 126.72   |
| 2   | N     | 301 | ADP  | C5-C4-N3 | -5.66 | 118.92      | 126.72   |
| 2   | U     | 301 | ADP  | N3-C4-N9 | 4.32  | 134.52      | 127.17   |
| 2   | H     | 301 | ADP  | N3-C4-N9 | 4.32  | 134.51      | 127.17   |
| 2   | l     | 301 | ADP  | N3-C4-N9 | 4.31  | 134.50      | 127.17   |
| 2   | K     | 301 | ADP  | N3-C4-N9 | 4.31  | 134.50      | 127.17   |
| 2   | x     | 301 | ADP  | N3-C4-N9 | 4.31  | 134.50      | 127.17   |
| 2   | 3     | 301 | ADP  | N3-C4-N9 | 4.31  | 134.49      | 127.17   |
| 2   | D     | 301 | ADP  | N3-C4-N9 | 4.31  | 134.49      | 127.17   |
| 2   | L     | 301 | ADP  | N3-C4-N9 | 4.30  | 134.49      | 127.17   |
| 2   | c     | 301 | ADP  | N3-C4-N9 | 4.30  | 134.49      | 127.17   |
| 2   | W     | 301 | ADP  | N3-C4-N9 | 4.30  | 134.48      | 127.17   |
| 2   | V     | 301 | ADP  | N3-C4-N9 | 4.30  | 134.48      | 127.17   |
| 2   | Z     | 301 | ADP  | N3-C4-N9 | 4.30  | 134.48      | 127.17   |
| 2   | k     | 301 | ADP  | N3-C4-N9 | 4.30  | 134.48      | 127.17   |
| 2   | e     | 301 | ADP  | N3-C4-N9 | 4.30  | 134.48      | 127.17   |
| 2   | C     | 301 | ADP  | N3-C4-N9 | 4.30  | 134.47      | 127.17   |
| 2   | b     | 301 | ADP  | N3-C4-N9 | 4.30  | 134.47      | 127.17   |
| 2   | z     | 301 | ADP  | N3-C4-N9 | 4.29  | 134.47      | 127.17   |
| 2   | 7     | 301 | ADP  | N3-C4-N9 | 4.29  | 134.47      | 127.17   |
| 2   | G     | 301 | ADP  | N3-C4-N9 | 4.29  | 134.47      | 127.17   |
| 2   | r     | 301 | ADP  | N3-C4-N9 | 4.29  | 134.47      | 127.17   |
| 2   | X     | 301 | ADP  | N3-C4-N9 | 4.29  | 134.47      | 127.17   |
| 2   | Q     | 301 | ADP  | N3-C4-N9 | 4.29  | 134.47      | 127.17   |
| 2   | T     | 301 | ADP  | N3-C4-N9 | 4.29  | 134.46      | 127.17   |
| 2   | d     | 301 | ADP  | N3-C4-N9 | 4.29  | 134.46      | 127.17   |
| 2   | Y     | 301 | ADP  | N3-C4-N9 | 4.29  | 134.46      | 127.17   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2   | v     | 301 | ADP  | N3-C4-N9 | 4.29 | 134.46      | 127.17   |
| 2   | P     | 301 | ADP  | N3-C4-N9 | 4.29 | 134.46      | 127.17   |
| 2   | M     | 301 | ADP  | N3-C4-N9 | 4.28 | 134.45      | 127.17   |
| 2   | a     | 301 | ADP  | N3-C4-N9 | 4.28 | 134.45      | 127.17   |
| 2   | i     | 301 | ADP  | N3-C4-N9 | 4.28 | 134.45      | 127.17   |
| 2   | p     | 301 | ADP  | N3-C4-N9 | 4.28 | 134.45      | 127.17   |
| 2   | 6     | 301 | ADP  | N3-C4-N9 | 4.28 | 134.45      | 127.17   |
| 2   | B     | 301 | ADP  | N3-C4-N9 | 4.28 | 134.45      | 127.17   |
| 2   | I     | 301 | ADP  | N3-C4-N9 | 4.28 | 134.45      | 127.17   |
| 2   | S     | 301 | ADP  | N3-C4-N9 | 4.28 | 134.45      | 127.17   |
| 2   | 5     | 301 | ADP  | N3-C4-N9 | 4.28 | 134.45      | 127.17   |
| 2   | m     | 301 | ADP  | N3-C4-N9 | 4.28 | 134.45      | 127.17   |
| 2   | o     | 301 | ADP  | N3-C4-N9 | 4.28 | 134.44      | 127.17   |
| 2   | j     | 301 | ADP  | N3-C4-N9 | 4.28 | 134.44      | 127.17   |
| 2   | 4     | 301 | ADP  | N3-C4-N9 | 4.28 | 134.44      | 127.17   |
| 2   | 0     | 301 | ADP  | N3-C4-N9 | 4.27 | 134.44      | 127.17   |
| 2   | n     | 301 | ADP  | N3-C4-N9 | 4.27 | 134.44      | 127.17   |
| 2   | F     | 301 | ADP  | N3-C4-N9 | 4.27 | 134.44      | 127.17   |
| 2   | E     | 301 | ADP  | N3-C4-N9 | 4.27 | 134.43      | 127.17   |
| 2   | u     | 301 | ADP  | N3-C4-N9 | 4.27 | 134.43      | 127.17   |
| 2   | A     | 301 | ADP  | N3-C4-N9 | 4.27 | 134.43      | 127.17   |
| 2   | q     | 301 | ADP  | N3-C4-N9 | 4.27 | 134.43      | 127.17   |
| 2   | w     | 301 | ADP  | N3-C4-N9 | 4.27 | 134.43      | 127.17   |
| 2   | y     | 301 | ADP  | N3-C4-N9 | 4.27 | 134.43      | 127.17   |
| 2   | R     | 301 | ADP  | N3-C4-N9 | 4.27 | 134.43      | 127.17   |
| 2   | J     | 301 | ADP  | N3-C4-N9 | 4.27 | 134.42      | 127.17   |
| 2   | h     | 301 | ADP  | N3-C4-N9 | 4.27 | 134.42      | 127.17   |
| 2   | l     | 301 | ADP  | N3-C4-N9 | 4.26 | 134.42      | 127.17   |
| 2   | f     | 301 | ADP  | N3-C4-N9 | 4.26 | 134.42      | 127.17   |
| 2   | s     | 301 | ADP  | N3-C4-N9 | 4.26 | 134.41      | 127.17   |
| 2   | N     | 301 | ADP  | N3-C4-N9 | 4.26 | 134.41      | 127.17   |
| 2   | O     | 301 | ADP  | N3-C4-N9 | 4.26 | 134.40      | 127.17   |
| 2   | t     | 301 | ADP  | N3-C4-N9 | 4.25 | 134.40      | 127.17   |
| 2   | g     | 301 | ADP  | N3-C4-N9 | 4.24 | 134.39      | 127.17   |
| 2   | 2     | 301 | ADP  | N3-C4-N9 | 4.24 | 134.38      | 127.17   |
| 2   | 6     | 301 | ADP  | C2-N3-C4 | 3.88 | 121.31      | 111.83   |
| 2   | K     | 301 | ADP  | C2-N3-C4 | 3.88 | 121.31      | 111.83   |
| 2   | U     | 301 | ADP  | C2-N3-C4 | 3.88 | 121.30      | 111.83   |
| 2   | Z     | 301 | ADP  | C2-N3-C4 | 3.87 | 121.29      | 111.83   |
| 2   | d     | 301 | ADP  | C2-N3-C4 | 3.87 | 121.29      | 111.83   |
| 2   | i     | 301 | ADP  | C2-N3-C4 | 3.87 | 121.29      | 111.83   |
| 2   | 3     | 301 | ADP  | C2-N3-C4 | 3.87 | 121.28      | 111.83   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2   | V     | 301 | ADP  | C2-N3-C4 | 3.87 | 121.28      | 111.83   |
| 2   | Q     | 301 | ADP  | C2-N3-C4 | 3.87 | 121.28      | 111.83   |
| 2   | k     | 301 | ADP  | C2-N3-C4 | 3.87 | 121.28      | 111.83   |
| 2   | L     | 301 | ADP  | C2-N3-C4 | 3.87 | 121.28      | 111.83   |
| 2   | I     | 301 | ADP  | C2-N3-C4 | 3.87 | 121.28      | 111.83   |
| 2   | n     | 301 | ADP  | C2-N3-C4 | 3.87 | 121.28      | 111.83   |
| 2   | y     | 301 | ADP  | C2-N3-C4 | 3.87 | 121.28      | 111.83   |
| 2   | H     | 301 | ADP  | C2-N3-C4 | 3.87 | 121.28      | 111.83   |
| 2   | a     | 301 | ADP  | C2-N3-C4 | 3.87 | 121.28      | 111.83   |
| 2   | C     | 301 | ADP  | C2-N3-C4 | 3.87 | 121.27      | 111.83   |
| 2   | P     | 301 | ADP  | C2-N3-C4 | 3.87 | 121.27      | 111.83   |
| 2   | W     | 301 | ADP  | C2-N3-C4 | 3.86 | 121.27      | 111.83   |
| 2   | b     | 301 | ADP  | C2-N3-C4 | 3.86 | 121.27      | 111.83   |
| 2   | m     | 301 | ADP  | C2-N3-C4 | 3.86 | 121.27      | 111.83   |
| 2   | 5     | 301 | ADP  | C2-N3-C4 | 3.86 | 121.27      | 111.83   |
| 2   | s     | 301 | ADP  | C2-N3-C4 | 3.86 | 121.27      | 111.83   |
| 2   | 0     | 301 | ADP  | C2-N3-C4 | 3.86 | 121.27      | 111.83   |
| 2   | x     | 301 | ADP  | C2-N3-C4 | 3.86 | 121.26      | 111.83   |
| 2   | G     | 301 | ADP  | C2-N3-C4 | 3.86 | 121.26      | 111.83   |
| 2   | T     | 301 | ADP  | C2-N3-C4 | 3.86 | 121.26      | 111.83   |
| 2   | r     | 301 | ADP  | C2-N3-C4 | 3.86 | 121.26      | 111.83   |
| 2   | c     | 301 | ADP  | C2-N3-C4 | 3.86 | 121.26      | 111.83   |
| 2   | 7     | 301 | ADP  | C2-N3-C4 | 3.86 | 121.26      | 111.83   |
| 2   | o     | 301 | ADP  | C2-N3-C4 | 3.86 | 121.26      | 111.83   |
| 2   | R     | 301 | ADP  | C2-N3-C4 | 3.86 | 121.25      | 111.83   |
| 2   | J     | 301 | ADP  | C2-N3-C4 | 3.86 | 121.25      | 111.83   |
| 2   | D     | 301 | ADP  | C2-N3-C4 | 3.85 | 121.24      | 111.83   |
| 2   | X     | 301 | ADP  | C2-N3-C4 | 3.85 | 121.24      | 111.83   |
| 2   | q     | 301 | ADP  | C2-N3-C4 | 3.85 | 121.24      | 111.83   |
| 2   | 1     | 301 | ADP  | C2-N3-C4 | 3.85 | 121.24      | 111.83   |
| 2   | f     | 301 | ADP  | C2-N3-C4 | 3.85 | 121.24      | 111.83   |
| 2   | 4     | 301 | ADP  | C2-N3-C4 | 3.85 | 121.24      | 111.83   |
| 2   | u     | 301 | ADP  | C2-N3-C4 | 3.85 | 121.24      | 111.83   |
| 2   | v     | 301 | ADP  | C2-N3-C4 | 3.85 | 121.24      | 111.83   |
| 2   | 2     | 301 | ADP  | C2-N3-C4 | 3.85 | 121.24      | 111.83   |
| 2   | l     | 301 | ADP  | C2-N3-C4 | 3.85 | 121.24      | 111.83   |
| 2   | M     | 301 | ADP  | C2-N3-C4 | 3.85 | 121.23      | 111.83   |
| 2   | e     | 301 | ADP  | C2-N3-C4 | 3.85 | 121.23      | 111.83   |
| 2   | h     | 301 | ADP  | C2-N3-C4 | 3.85 | 121.23      | 111.83   |
| 2   | A     | 301 | ADP  | C2-N3-C4 | 3.85 | 121.23      | 111.83   |
| 2   | S     | 301 | ADP  | C2-N3-C4 | 3.85 | 121.23      | 111.83   |
| 2   | E     | 301 | ADP  | C2-N3-C4 | 3.85 | 121.23      | 111.83   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | p     | 301 | ADP  | C2-N3-C4 | 3.85  | 121.23      | 111.83   |
| 2   | z     | 301 | ADP  | C2-N3-C4 | 3.85  | 121.22      | 111.83   |
| 2   | F     | 301 | ADP  | C2-N3-C4 | 3.84  | 121.22      | 111.83   |
| 2   | w     | 301 | ADP  | C2-N3-C4 | 3.84  | 121.22      | 111.83   |
| 2   | Y     | 301 | ADP  | C2-N3-C4 | 3.84  | 121.22      | 111.83   |
| 2   | j     | 301 | ADP  | C2-N3-C4 | 3.84  | 121.22      | 111.83   |
| 2   | O     | 301 | ADP  | C2-N3-C4 | 3.84  | 121.22      | 111.83   |
| 2   | B     | 301 | ADP  | C2-N3-C4 | 3.84  | 121.21      | 111.83   |
| 2   | g     | 301 | ADP  | C2-N3-C4 | 3.84  | 121.21      | 111.83   |
| 2   | N     | 301 | ADP  | C2-N3-C4 | 3.84  | 121.20      | 111.83   |
| 2   | t     | 301 | ADP  | C2-N3-C4 | 3.84  | 121.20      | 111.83   |
| 2   | I     | 301 | ADP  | N3-C2-N1 | -3.82 | 122.79      | 128.58   |
| 2   | U     | 301 | ADP  | N3-C2-N1 | -3.82 | 122.80      | 128.58   |
| 2   | K     | 301 | ADP  | N3-C2-N1 | -3.82 | 122.80      | 128.58   |
| 2   | y     | 301 | ADP  | N3-C2-N1 | -3.82 | 122.81      | 128.58   |
| 2   | 6     | 301 | ADP  | N3-C2-N1 | -3.81 | 122.81      | 128.58   |
| 2   | 3     | 301 | ADP  | N3-C2-N1 | -3.81 | 122.82      | 128.58   |
| 2   | O     | 301 | ADP  | N3-C2-N1 | -3.81 | 122.82      | 128.58   |
| 2   | i     | 301 | ADP  | N3-C2-N1 | -3.81 | 122.82      | 128.58   |
| 2   | V     | 301 | ADP  | N3-C2-N1 | -3.81 | 122.82      | 128.58   |
| 2   | 1     | 301 | ADP  | N3-C2-N1 | -3.80 | 122.82      | 128.58   |
| 2   | a     | 301 | ADP  | N3-C2-N1 | -3.80 | 122.83      | 128.58   |
| 2   | F     | 301 | ADP  | N3-C2-N1 | -3.80 | 122.83      | 128.58   |
| 2   | d     | 301 | ADP  | N3-C2-N1 | -3.80 | 122.83      | 128.58   |
| 2   | 5     | 301 | ADP  | N3-C2-N1 | -3.80 | 122.83      | 128.58   |
| 2   | T     | 301 | ADP  | N3-C2-N1 | -3.80 | 122.83      | 128.58   |
| 2   | n     | 301 | ADP  | N3-C2-N1 | -3.80 | 122.83      | 128.58   |
| 2   | s     | 301 | ADP  | N3-C2-N1 | -3.80 | 122.83      | 128.58   |
| 2   | 0     | 301 | ADP  | N3-C2-N1 | -3.80 | 122.83      | 128.58   |
| 2   | j     | 301 | ADP  | N3-C2-N1 | -3.80 | 122.83      | 128.58   |
| 2   | u     | 301 | ADP  | N3-C2-N1 | -3.80 | 122.83      | 128.58   |
| 2   | c     | 301 | ADP  | N3-C2-N1 | -3.80 | 122.84      | 128.58   |
| 2   | 2     | 301 | ADP  | N3-C2-N1 | -3.80 | 122.84      | 128.58   |
| 2   | R     | 301 | ADP  | N3-C2-N1 | -3.79 | 122.84      | 128.58   |
| 2   | C     | 301 | ADP  | N3-C2-N1 | -3.79 | 122.84      | 128.58   |
| 2   | m     | 301 | ADP  | N3-C2-N1 | -3.79 | 122.84      | 128.58   |
| 2   | w     | 301 | ADP  | N3-C2-N1 | -3.79 | 122.84      | 128.58   |
| 2   | b     | 301 | ADP  | N3-C2-N1 | -3.79 | 122.84      | 128.58   |
| 2   | P     | 301 | ADP  | N3-C2-N1 | -3.79 | 122.84      | 128.58   |
| 2   | 4     | 301 | ADP  | N3-C2-N1 | -3.79 | 122.85      | 128.58   |
| 2   | Q     | 301 | ADP  | N3-C2-N1 | -3.79 | 122.85      | 128.58   |
| 2   | W     | 301 | ADP  | N3-C2-N1 | -3.79 | 122.85      | 128.58   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | N     | 301 | ADP  | N3-C2-N1 | -3.79 | 122.85      | 128.58   |
| 2   | Z     | 301 | ADP  | N3-C2-N1 | -3.79 | 122.85      | 128.58   |
| 2   | z     | 301 | ADP  | N3-C2-N1 | -3.79 | 122.85      | 128.58   |
| 2   | f     | 301 | ADP  | N3-C2-N1 | -3.79 | 122.85      | 128.58   |
| 2   | D     | 301 | ADP  | N3-C2-N1 | -3.78 | 122.85      | 128.58   |
| 2   | o     | 301 | ADP  | N3-C2-N1 | -3.78 | 122.85      | 128.58   |
| 2   | G     | 301 | ADP  | N3-C2-N1 | -3.78 | 122.86      | 128.58   |
| 2   | q     | 301 | ADP  | N3-C2-N1 | -3.78 | 122.86      | 128.58   |
| 2   | t     | 301 | ADP  | N3-C2-N1 | -3.78 | 122.86      | 128.58   |
| 2   | A     | 301 | ADP  | N3-C2-N1 | -3.78 | 122.86      | 128.58   |
| 2   | L     | 301 | ADP  | N3-C2-N1 | -3.78 | 122.86      | 128.58   |
| 2   | E     | 301 | ADP  | N3-C2-N1 | -3.78 | 122.86      | 128.58   |
| 2   | v     | 301 | ADP  | N3-C2-N1 | -3.78 | 122.86      | 128.58   |
| 2   | x     | 301 | ADP  | N3-C2-N1 | -3.78 | 122.86      | 128.58   |
| 2   | J     | 301 | ADP  | N3-C2-N1 | -3.78 | 122.86      | 128.58   |
| 2   | k     | 301 | ADP  | N3-C2-N1 | -3.78 | 122.87      | 128.58   |
| 2   | M     | 301 | ADP  | N3-C2-N1 | -3.78 | 122.87      | 128.58   |
| 2   | Y     | 301 | ADP  | N3-C2-N1 | -3.78 | 122.87      | 128.58   |
| 2   | r     | 301 | ADP  | N3-C2-N1 | -3.77 | 122.87      | 128.58   |
| 2   | S     | 301 | ADP  | N3-C2-N1 | -3.77 | 122.87      | 128.58   |
| 2   | H     | 301 | ADP  | N3-C2-N1 | -3.77 | 122.87      | 128.58   |
| 2   | e     | 301 | ADP  | N3-C2-N1 | -3.77 | 122.87      | 128.58   |
| 2   | p     | 301 | ADP  | N3-C2-N1 | -3.77 | 122.87      | 128.58   |
| 2   | X     | 301 | ADP  | N3-C2-N1 | -3.77 | 122.87      | 128.58   |
| 2   | 7     | 301 | ADP  | N3-C2-N1 | -3.77 | 122.88      | 128.58   |
| 2   | h     | 301 | ADP  | N3-C2-N1 | -3.77 | 122.88      | 128.58   |
| 2   | B     | 301 | ADP  | N3-C2-N1 | -3.77 | 122.88      | 128.58   |
| 2   | g     | 301 | ADP  | N3-C2-N1 | -3.76 | 122.88      | 128.58   |
| 2   | l     | 301 | ADP  | N3-C2-N1 | -3.76 | 122.89      | 128.58   |
| 2   | 6     | 301 | ADP  | C4-C5-N7 | -3.71 | 106.34      | 110.58   |
| 2   | 5     | 301 | ADP  | C4-C5-N7 | -3.71 | 106.34      | 110.58   |
| 2   | t     | 301 | ADP  | C4-C5-N7 | -3.70 | 106.36      | 110.58   |
| 2   | e     | 301 | ADP  | C4-C5-N7 | -3.69 | 106.36      | 110.58   |
| 2   | I     | 301 | ADP  | C4-C5-N7 | -3.69 | 106.36      | 110.58   |
| 2   | g     | 301 | ADP  | C4-C5-N7 | -3.69 | 106.37      | 110.58   |
| 2   | r     | 301 | ADP  | C4-C5-N7 | -3.68 | 106.37      | 110.58   |
| 2   | 0     | 301 | ADP  | C4-C5-N7 | -3.68 | 106.37      | 110.58   |
| 2   | V     | 301 | ADP  | C4-C5-N7 | -3.68 | 106.37      | 110.58   |
| 2   | 2     | 301 | ADP  | C4-C5-N7 | -3.68 | 106.37      | 110.58   |
| 2   | a     | 301 | ADP  | C4-C5-N7 | -3.68 | 106.37      | 110.58   |
| 2   | l     | 301 | ADP  | C4-C5-N7 | -3.68 | 106.37      | 110.58   |
| 2   | M     | 301 | ADP  | C4-C5-N7 | -3.68 | 106.38      | 110.58   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | p     | 301 | ADP  | C4-C5-N7 | -3.68 | 106.38      | 110.58   |
| 2   | 4     | 301 | ADP  | C4-C5-N7 | -3.67 | 106.38      | 110.58   |
| 2   | P     | 301 | ADP  | C4-C5-N7 | -3.67 | 106.38      | 110.58   |
| 2   | Q     | 301 | ADP  | C4-C5-N7 | -3.67 | 106.38      | 110.58   |
| 2   | 3     | 301 | ADP  | C4-C5-N7 | -3.67 | 106.39      | 110.58   |
| 2   | k     | 301 | ADP  | C4-C5-N7 | -3.67 | 106.39      | 110.58   |
| 2   | N     | 301 | ADP  | C4-C5-N7 | -3.67 | 106.39      | 110.58   |
| 2   | z     | 301 | ADP  | C4-C5-N7 | -3.67 | 106.39      | 110.58   |
| 2   | q     | 301 | ADP  | C4-C5-N7 | -3.66 | 106.39      | 110.58   |
| 2   | 7     | 301 | ADP  | C4-C5-N7 | -3.66 | 106.40      | 110.58   |
| 2   | Z     | 301 | ADP  | C4-C5-N7 | -3.66 | 106.40      | 110.58   |
| 2   | d     | 301 | ADP  | C4-C5-N7 | -3.66 | 106.40      | 110.58   |
| 2   | n     | 301 | ADP  | C4-C5-N7 | -3.66 | 106.40      | 110.58   |
| 2   | x     | 301 | ADP  | C4-C5-N7 | -3.66 | 106.40      | 110.58   |
| 2   | v     | 301 | ADP  | C4-C5-N7 | -3.66 | 106.40      | 110.58   |
| 2   | l     | 301 | ADP  | C4-C5-N7 | -3.66 | 106.40      | 110.58   |
| 2   | H     | 301 | ADP  | C4-C5-N7 | -3.65 | 106.40      | 110.58   |
| 2   | U     | 301 | ADP  | C4-C5-N7 | -3.65 | 106.40      | 110.58   |
| 2   | b     | 301 | ADP  | C4-C5-N7 | -3.65 | 106.40      | 110.58   |
| 2   | h     | 301 | ADP  | C4-C5-N7 | -3.65 | 106.41      | 110.58   |
| 2   | X     | 301 | ADP  | C4-C5-N7 | -3.65 | 106.41      | 110.58   |
| 2   | G     | 301 | ADP  | C4-C5-N7 | -3.65 | 106.41      | 110.58   |
| 2   | o     | 301 | ADP  | C4-C5-N7 | -3.65 | 106.41      | 110.58   |
| 2   | O     | 301 | ADP  | C4-C5-N7 | -3.65 | 106.41      | 110.58   |
| 2   | R     | 301 | ADP  | C4-C5-N7 | -3.65 | 106.41      | 110.58   |
| 2   | y     | 301 | ADP  | C4-C5-N7 | -3.65 | 106.41      | 110.58   |
| 2   | B     | 301 | ADP  | C4-C5-N7 | -3.65 | 106.41      | 110.58   |
| 2   | J     | 301 | ADP  | C4-C5-N7 | -3.65 | 106.41      | 110.58   |
| 2   | D     | 301 | ADP  | C4-C5-N7 | -3.65 | 106.41      | 110.58   |
| 2   | s     | 301 | ADP  | C4-C5-N7 | -3.65 | 106.41      | 110.58   |
| 2   | E     | 301 | ADP  | C4-C5-N7 | -3.64 | 106.42      | 110.58   |
| 2   | W     | 301 | ADP  | C4-C5-N7 | -3.64 | 106.42      | 110.58   |
| 2   | S     | 301 | ADP  | C4-C5-N7 | -3.64 | 106.42      | 110.58   |
| 2   | Y     | 301 | ADP  | C4-C5-N7 | -3.64 | 106.42      | 110.58   |
| 2   | f     | 301 | ADP  | C4-C5-N7 | -3.64 | 106.42      | 110.58   |
| 2   | F     | 301 | ADP  | C4-C5-N7 | -3.64 | 106.42      | 110.58   |
| 2   | m     | 301 | ADP  | C4-C5-N7 | -3.64 | 106.42      | 110.58   |
| 2   | w     | 301 | ADP  | C4-C5-N7 | -3.64 | 106.42      | 110.58   |
| 2   | i     | 301 | ADP  | C4-C5-N7 | -3.64 | 106.42      | 110.58   |
| 2   | K     | 301 | ADP  | C4-C5-N7 | -3.63 | 106.43      | 110.58   |
| 2   | c     | 301 | ADP  | C4-C5-N7 | -3.63 | 106.43      | 110.58   |
| 2   | C     | 301 | ADP  | C4-C5-N7 | -3.63 | 106.43      | 110.58   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | j     | 301 | ADP  | C4-C5-N7 | -3.63 | 106.44      | 110.58   |
| 2   | u     | 301 | ADP  | C4-C5-N7 | -3.62 | 106.44      | 110.58   |
| 2   | A     | 301 | ADP  | C4-C5-N7 | -3.62 | 106.44      | 110.58   |
| 2   | T     | 301 | ADP  | C4-C5-N7 | -3.62 | 106.44      | 110.58   |
| 2   | L     | 301 | ADP  | C4-C5-N7 | -3.61 | 106.45      | 110.58   |
| 2   | N     | 301 | ADP  | C5-N7-C8 | 2.77  | 107.80      | 103.45   |
| 2   | 6     | 301 | ADP  | C5-N7-C8 | 2.76  | 107.79      | 103.45   |
| 2   | g     | 301 | ADP  | C5-N7-C8 | 2.76  | 107.78      | 103.45   |
| 2   | e     | 301 | ADP  | C5-N7-C8 | 2.75  | 107.78      | 103.45   |
| 2   | a     | 301 | ADP  | C5-N7-C8 | 2.75  | 107.77      | 103.45   |
| 2   | G     | 301 | ADP  | C5-N7-C8 | 2.75  | 107.77      | 103.45   |
| 2   | r     | 301 | ADP  | C5-N7-C8 | 2.75  | 107.77      | 103.45   |
| 2   | M     | 301 | ADP  | C5-N7-C8 | 2.75  | 107.77      | 103.45   |
| 2   | Y     | 301 | ADP  | C5-N7-C8 | 2.75  | 107.77      | 103.45   |
| 2   | p     | 301 | ADP  | C5-N7-C8 | 2.74  | 107.76      | 103.45   |
| 2   | 7     | 301 | ADP  | C5-N7-C8 | 2.74  | 107.76      | 103.45   |
| 2   | k     | 301 | ADP  | C5-N7-C8 | 2.74  | 107.76      | 103.45   |
| 2   | S     | 301 | ADP  | C5-N7-C8 | 2.74  | 107.76      | 103.45   |
| 2   | y     | 301 | ADP  | C5-N7-C8 | 2.74  | 107.76      | 103.45   |
| 2   | E     | 301 | ADP  | C5-N7-C8 | 2.74  | 107.76      | 103.45   |
| 2   | w     | 301 | ADP  | C5-N7-C8 | 2.74  | 107.76      | 103.45   |
| 2   | I     | 301 | ADP  | C5-N7-C8 | 2.74  | 107.75      | 103.45   |
| 2   | f     | 301 | ADP  | C5-N7-C8 | 2.74  | 107.75      | 103.45   |
| 2   | m     | 301 | ADP  | C5-N7-C8 | 2.74  | 107.75      | 103.45   |
| 2   | 5     | 301 | ADP  | C5-N7-C8 | 2.74  | 107.75      | 103.45   |
| 2   | z     | 301 | ADP  | C5-N7-C8 | 2.73  | 107.75      | 103.45   |
| 2   | 0     | 301 | ADP  | C5-N7-C8 | 2.73  | 107.75      | 103.45   |
| 2   | B     | 301 | ADP  | C5-N7-C8 | 2.73  | 107.75      | 103.45   |
| 2   | O     | 301 | ADP  | C5-N7-C8 | 2.73  | 107.75      | 103.45   |
| 2   | t     | 301 | ADP  | C5-N7-C8 | 2.73  | 107.75      | 103.45   |
| 2   | U     | 301 | ADP  | C5-N7-C8 | 2.73  | 107.75      | 103.45   |
| 2   | X     | 301 | ADP  | C5-N7-C8 | 2.73  | 107.74      | 103.45   |
| 2   | j     | 301 | ADP  | C5-N7-C8 | 2.73  | 107.74      | 103.45   |
| 2   | l     | 301 | ADP  | C5-N7-C8 | 2.73  | 107.74      | 103.45   |
| 2   | o     | 301 | ADP  | C5-N7-C8 | 2.73  | 107.74      | 103.45   |
| 2   | q     | 301 | ADP  | C5-N7-C8 | 2.73  | 107.74      | 103.45   |
| 2   | D     | 301 | ADP  | C5-N7-C8 | 2.73  | 107.74      | 103.45   |
| 2   | P     | 301 | ADP  | C5-N7-C8 | 2.73  | 107.74      | 103.45   |
| 2   | 4     | 301 | ADP  | C5-N7-C8 | 2.73  | 107.74      | 103.45   |
| 2   | Q     | 301 | ADP  | C5-N7-C8 | 2.73  | 107.74      | 103.45   |
| 2   | s     | 301 | ADP  | C5-N7-C8 | 2.73  | 107.74      | 103.45   |
| 2   | x     | 301 | ADP  | C5-N7-C8 | 2.73  | 107.74      | 103.45   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2   | V     | 301 | ADP  | C5-N7-C8 | 2.73 | 107.74      | 103.45   |
| 2   | 3     | 301 | ADP  | C5-N7-C8 | 2.73 | 107.73      | 103.45   |
| 2   | u     | 301 | ADP  | C5-N7-C8 | 2.73 | 107.73      | 103.45   |
| 2   | b     | 301 | ADP  | C5-N7-C8 | 2.73 | 107.73      | 103.45   |
| 2   | 2     | 301 | ADP  | C5-N7-C8 | 2.73 | 107.73      | 103.45   |
| 2   | J     | 301 | ADP  | C5-N7-C8 | 2.73 | 107.73      | 103.45   |
| 2   | T     | 301 | ADP  | C5-N7-C8 | 2.72 | 107.73      | 103.45   |
| 2   | Z     | 301 | ADP  | C5-N7-C8 | 2.72 | 107.73      | 103.45   |
| 2   | F     | 301 | ADP  | C5-N7-C8 | 2.72 | 107.72      | 103.45   |
| 2   | c     | 301 | ADP  | C5-N7-C8 | 2.72 | 107.72      | 103.45   |
| 2   | h     | 301 | ADP  | C5-N7-C8 | 2.72 | 107.72      | 103.45   |
| 2   | n     | 301 | ADP  | C5-N7-C8 | 2.72 | 107.72      | 103.45   |
| 2   | W     | 301 | ADP  | C5-N7-C8 | 2.72 | 107.72      | 103.45   |
| 2   | L     | 301 | ADP  | C5-N7-C8 | 2.72 | 107.72      | 103.45   |
| 2   | R     | 301 | ADP  | C5-N7-C8 | 2.71 | 107.71      | 103.45   |
| 2   | i     | 301 | ADP  | C5-N7-C8 | 2.71 | 107.71      | 103.45   |
| 2   | C     | 301 | ADP  | C5-N7-C8 | 2.71 | 107.71      | 103.45   |
| 2   | K     | 301 | ADP  | C5-N7-C8 | 2.71 | 107.71      | 103.45   |
| 2   | 1     | 301 | ADP  | C5-N7-C8 | 2.71 | 107.71      | 103.45   |
| 2   | H     | 301 | ADP  | C5-N7-C8 | 2.71 | 107.70      | 103.45   |
| 2   | d     | 301 | ADP  | C5-N7-C8 | 2.70 | 107.70      | 103.45   |
| 2   | A     | 301 | ADP  | C5-N7-C8 | 2.70 | 107.69      | 103.45   |
| 2   | v     | 301 | ADP  | C5-N7-C8 | 2.70 | 107.69      | 103.45   |
| 2   | l     | 301 | ADP  | C4-N9-C8 | 2.60 | 108.46      | 105.74   |
| 2   | H     | 301 | ADP  | C4-N9-C8 | 2.57 | 108.44      | 105.74   |
| 2   | B     | 301 | ADP  | C4-N9-C8 | 2.56 | 108.42      | 105.74   |
| 2   | U     | 301 | ADP  | C4-N9-C8 | 2.56 | 108.42      | 105.74   |
| 2   | D     | 301 | ADP  | C4-N9-C8 | 2.55 | 108.42      | 105.74   |
| 2   | e     | 301 | ADP  | C4-N9-C8 | 2.55 | 108.42      | 105.74   |
| 2   | L     | 301 | ADP  | C4-N9-C8 | 2.55 | 108.42      | 105.74   |
| 2   | k     | 301 | ADP  | C4-N9-C8 | 2.55 | 108.42      | 105.74   |
| 2   | 3     | 301 | ADP  | C4-N9-C8 | 2.55 | 108.41      | 105.74   |
| 2   | F     | 301 | ADP  | C4-N9-C8 | 2.55 | 108.41      | 105.74   |
| 2   | Z     | 301 | ADP  | C4-N9-C8 | 2.54 | 108.41      | 105.74   |
| 2   | W     | 301 | ADP  | C4-N9-C8 | 2.54 | 108.41      | 105.74   |
| 2   | c     | 301 | ADP  | C4-N9-C8 | 2.54 | 108.40      | 105.74   |
| 2   | z     | 301 | ADP  | C4-N9-C8 | 2.54 | 108.40      | 105.74   |
| 2   | r     | 301 | ADP  | C4-N9-C8 | 2.54 | 108.40      | 105.74   |
| 2   | 7     | 301 | ADP  | C4-N9-C8 | 2.54 | 108.40      | 105.74   |
| 2   | M     | 301 | ADP  | C4-N9-C8 | 2.53 | 108.40      | 105.74   |
| 2   | T     | 301 | ADP  | C4-N9-C8 | 2.53 | 108.40      | 105.74   |
| 2   | Y     | 301 | ADP  | C4-N9-C8 | 2.53 | 108.40      | 105.74   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2   | p     | 301 | ADP  | C4-N9-C8 | 2.53 | 108.40      | 105.74   |
| 2   | u     | 301 | ADP  | C4-N9-C8 | 2.53 | 108.39      | 105.74   |
| 2   | q     | 301 | ADP  | C4-N9-C8 | 2.53 | 108.39      | 105.74   |
| 2   | x     | 301 | ADP  | C4-N9-C8 | 2.53 | 108.39      | 105.74   |
| 2   | S     | 301 | ADP  | C4-N9-C8 | 2.53 | 108.39      | 105.74   |
| 2   | C     | 301 | ADP  | C4-N9-C8 | 2.52 | 108.39      | 105.74   |
| 2   | X     | 301 | ADP  | C4-N9-C8 | 2.52 | 108.39      | 105.74   |
| 2   | E     | 301 | ADP  | C4-N9-C8 | 2.52 | 108.39      | 105.74   |
| 2   | V     | 301 | ADP  | C4-N9-C8 | 2.52 | 108.39      | 105.74   |
| 2   | j     | 301 | ADP  | C4-N9-C8 | 2.52 | 108.39      | 105.74   |
| 2   | b     | 301 | ADP  | C4-N9-C8 | 2.52 | 108.39      | 105.74   |
| 2   | R     | 301 | ADP  | C4-N9-C8 | 2.52 | 108.38      | 105.74   |
| 2   | O     | 301 | ADP  | C4-N9-C8 | 2.52 | 108.38      | 105.74   |
| 2   | v     | 301 | ADP  | C4-N9-C8 | 2.52 | 108.38      | 105.74   |
| 2   | 4     | 301 | ADP  | C4-N9-C8 | 2.52 | 108.38      | 105.74   |
| 2   | o     | 301 | ADP  | C4-N9-C8 | 2.52 | 108.38      | 105.74   |
| 2   | t     | 301 | ADP  | C4-N9-C8 | 2.52 | 108.38      | 105.74   |
| 2   | K     | 301 | ADP  | C4-N9-C8 | 2.51 | 108.38      | 105.74   |
| 2   | A     | 301 | ADP  | C4-N9-C8 | 2.51 | 108.38      | 105.74   |
| 2   | w     | 301 | ADP  | C4-N9-C8 | 2.51 | 108.38      | 105.74   |
| 2   | 5     | 301 | ADP  | C4-N9-C8 | 2.51 | 108.37      | 105.74   |
| 2   | P     | 301 | ADP  | C4-N9-C8 | 2.51 | 108.37      | 105.74   |
| 2   | G     | 301 | ADP  | C4-N9-C8 | 2.50 | 108.36      | 105.74   |
| 2   | d     | 301 | ADP  | C4-N9-C8 | 2.50 | 108.36      | 105.74   |
| 2   | Q     | 301 | ADP  | C4-N9-C8 | 2.50 | 108.36      | 105.74   |
| 2   | s     | 301 | ADP  | C4-N9-C8 | 2.50 | 108.36      | 105.74   |
| 2   | I     | 301 | ADP  | C4-N9-C8 | 2.49 | 108.36      | 105.74   |
| 2   | 6     | 301 | ADP  | C4-N9-C8 | 2.49 | 108.35      | 105.74   |
| 2   | g     | 301 | ADP  | C4-N9-C8 | 2.49 | 108.35      | 105.74   |
| 2   | N     | 301 | ADP  | C4-N9-C8 | 2.49 | 108.35      | 105.74   |
| 2   | m     | 301 | ADP  | C4-N9-C8 | 2.49 | 108.35      | 105.74   |
| 2   | 0     | 301 | ADP  | C4-N9-C8 | 2.49 | 108.35      | 105.74   |
| 2   | a     | 301 | ADP  | C4-N9-C8 | 2.49 | 108.35      | 105.74   |
| 2   | f     | 301 | ADP  | C4-N9-C8 | 2.49 | 108.35      | 105.74   |
| 2   | i     | 301 | ADP  | C4-N9-C8 | 2.48 | 108.35      | 105.74   |
| 2   | 1     | 301 | ADP  | C4-N9-C8 | 2.48 | 108.34      | 105.74   |
| 2   | y     | 301 | ADP  | C4-N9-C8 | 2.48 | 108.34      | 105.74   |
| 2   | h     | 301 | ADP  | C4-N9-C8 | 2.48 | 108.34      | 105.74   |
| 2   | J     | 301 | ADP  | C4-N9-C8 | 2.47 | 108.33      | 105.74   |
| 2   | n     | 301 | ADP  | C4-N9-C8 | 2.47 | 108.33      | 105.74   |
| 2   | 2     | 301 | ADP  | C4-N9-C8 | 2.46 | 108.32      | 105.74   |
| 2   | N     | 301 | ADP  | C6-C5-N7 | 2.38 | 136.68      | 132.09   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2   | 5     | 301 | ADP  | C6-C5-N7 | 2.37 | 136.66      | 132.09   |
| 2   | a     | 301 | ADP  | C6-C5-N7 | 2.37 | 136.66      | 132.09   |
| 2   | 4     | 301 | ADP  | C6-C5-N7 | 2.37 | 136.65      | 132.09   |
| 2   | 6     | 301 | ADP  | C6-C5-N7 | 2.37 | 136.65      | 132.09   |
| 2   | z     | 301 | ADP  | C6-C5-N7 | 2.37 | 136.65      | 132.09   |
| 2   | I     | 301 | ADP  | C6-C5-N7 | 2.36 | 136.65      | 132.09   |
| 2   | e     | 301 | ADP  | C6-C5-N7 | 2.36 | 136.65      | 132.09   |
| 2   | V     | 301 | ADP  | C6-C5-N7 | 2.36 | 136.64      | 132.09   |
| 2   | 7     | 301 | ADP  | C6-C5-N7 | 2.36 | 136.64      | 132.09   |
| 2   | k     | 301 | ADP  | C6-C5-N7 | 2.36 | 136.64      | 132.09   |
| 2   | D     | 301 | ADP  | C6-C5-N7 | 2.36 | 136.63      | 132.09   |
| 2   | j     | 301 | ADP  | C6-C5-N7 | 2.35 | 136.63      | 132.09   |
| 2   | O     | 301 | ADP  | C6-C5-N7 | 2.35 | 136.63      | 132.09   |
| 2   | Y     | 301 | ADP  | C6-C5-N7 | 2.35 | 136.63      | 132.09   |
| 2   | G     | 301 | ADP  | C6-C5-N7 | 2.35 | 136.62      | 132.09   |
| 2   | 2     | 301 | ADP  | C6-C5-N7 | 2.35 | 136.62      | 132.09   |
| 2   | 0     | 301 | ADP  | C6-C5-N7 | 2.35 | 136.62      | 132.09   |
| 2   | U     | 301 | ADP  | C6-C5-N7 | 2.35 | 136.62      | 132.09   |
| 2   | f     | 301 | ADP  | C6-C5-N7 | 2.35 | 136.62      | 132.09   |
| 2   | E     | 301 | ADP  | C6-C5-N7 | 2.35 | 136.62      | 132.09   |
| 2   | r     | 301 | ADP  | C6-C5-N7 | 2.35 | 136.62      | 132.09   |
| 2   | g     | 301 | ADP  | C6-C5-N7 | 2.35 | 136.61      | 132.09   |
| 2   | t     | 301 | ADP  | C6-C5-N7 | 2.35 | 136.61      | 132.09   |
| 2   | W     | 301 | ADP  | C6-C5-N7 | 2.35 | 136.61      | 132.09   |
| 2   | K     | 301 | ADP  | C6-C5-N7 | 2.35 | 136.61      | 132.09   |
| 2   | h     | 301 | ADP  | C6-C5-N7 | 2.35 | 136.61      | 132.09   |
| 2   | F     | 301 | ADP  | C6-C5-N7 | 2.35 | 136.61      | 132.09   |
| 2   | l     | 301 | ADP  | C6-C5-N7 | 2.34 | 136.61      | 132.09   |
| 2   | C     | 301 | ADP  | C6-C5-N7 | 2.34 | 136.61      | 132.09   |
| 2   | Z     | 301 | ADP  | C6-C5-N7 | 2.34 | 136.61      | 132.09   |
| 2   | X     | 301 | ADP  | C6-C5-N7 | 2.34 | 136.61      | 132.09   |
| 2   | v     | 301 | ADP  | C6-C5-N7 | 2.34 | 136.60      | 132.09   |
| 2   | H     | 301 | ADP  | C6-C5-N7 | 2.34 | 136.60      | 132.09   |
| 2   | Q     | 301 | ADP  | C6-C5-N7 | 2.34 | 136.60      | 132.09   |
| 2   | w     | 301 | ADP  | C6-C5-N7 | 2.34 | 136.60      | 132.09   |
| 2   | i     | 301 | ADP  | C6-C5-N7 | 2.34 | 136.60      | 132.09   |
| 2   | x     | 301 | ADP  | C6-C5-N7 | 2.34 | 136.60      | 132.09   |
| 2   | 3     | 301 | ADP  | C6-C5-N7 | 2.34 | 136.59      | 132.09   |
| 2   | p     | 301 | ADP  | C6-C5-N7 | 2.34 | 136.59      | 132.09   |
| 2   | 1     | 301 | ADP  | C6-C5-N7 | 2.34 | 136.59      | 132.09   |
| 2   | M     | 301 | ADP  | C6-C5-N7 | 2.34 | 136.59      | 132.09   |
| 2   | A     | 301 | ADP  | C6-C5-N7 | 2.33 | 136.59      | 132.09   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | S     | 301 | ADP  | C6-C5-N7 | 2.33  | 136.59      | 132.09   |
| 2   | o     | 301 | ADP  | C6-C5-N7 | 2.33  | 136.59      | 132.09   |
| 2   | y     | 301 | ADP  | C6-C5-N7 | 2.33  | 136.59      | 132.09   |
| 2   | d     | 301 | ADP  | C6-C5-N7 | 2.33  | 136.59      | 132.09   |
| 2   | s     | 301 | ADP  | C6-C5-N7 | 2.33  | 136.59      | 132.09   |
| 2   | J     | 301 | ADP  | C6-C5-N7 | 2.33  | 136.59      | 132.09   |
| 2   | n     | 301 | ADP  | C6-C5-N7 | 2.33  | 136.59      | 132.09   |
| 2   | P     | 301 | ADP  | C6-C5-N7 | 2.33  | 136.59      | 132.09   |
| 2   | b     | 301 | ADP  | C6-C5-N7 | 2.33  | 136.59      | 132.09   |
| 2   | q     | 301 | ADP  | C6-C5-N7 | 2.33  | 136.58      | 132.09   |
| 2   | m     | 301 | ADP  | C6-C5-N7 | 2.33  | 136.58      | 132.09   |
| 2   | T     | 301 | ADP  | C6-C5-N7 | 2.32  | 136.57      | 132.09   |
| 2   | L     | 301 | ADP  | C6-C5-N7 | 2.32  | 136.57      | 132.09   |
| 2   | u     | 301 | ADP  | C6-C5-N7 | 2.32  | 136.57      | 132.09   |
| 2   | R     | 301 | ADP  | C6-C5-N7 | 2.32  | 136.57      | 132.09   |
| 2   | B     | 301 | ADP  | C6-C5-N7 | 2.32  | 136.56      | 132.09   |
| 2   | c     | 301 | ADP  | C6-C5-N7 | 2.31  | 136.55      | 132.09   |
| 2   | B     | 301 | ADP  | N9-C8-N7 | -2.26 | 110.73      | 113.94   |
| 2   | p     | 301 | ADP  | N9-C8-N7 | -2.26 | 110.73      | 113.94   |
| 2   | q     | 301 | ADP  | N9-C8-N7 | -2.25 | 110.74      | 113.94   |
| 2   | l     | 301 | ADP  | N9-C8-N7 | -2.25 | 110.74      | 113.94   |
| 2   | S     | 301 | ADP  | N9-C8-N7 | -2.25 | 110.74      | 113.94   |
| 2   | u     | 301 | ADP  | N9-C8-N7 | -2.25 | 110.75      | 113.94   |
| 2   | M     | 301 | ADP  | N9-C8-N7 | -2.25 | 110.75      | 113.94   |
| 2   | g     | 301 | ADP  | N9-C8-N7 | -2.25 | 110.75      | 113.94   |
| 2   | w     | 301 | ADP  | N9-C8-N7 | -2.25 | 110.75      | 113.94   |
| 2   | r     | 301 | ADP  | N9-C8-N7 | -2.25 | 110.75      | 113.94   |
| 2   | L     | 301 | ADP  | N9-C8-N7 | -2.24 | 110.75      | 113.94   |
| 2   | e     | 301 | ADP  | N9-C8-N7 | -2.24 | 110.75      | 113.94   |
| 2   | t     | 301 | ADP  | N9-C8-N7 | -2.24 | 110.75      | 113.94   |
| 2   | o     | 301 | ADP  | N9-C8-N7 | -2.24 | 110.76      | 113.94   |
| 2   | 3     | 301 | ADP  | N9-C8-N7 | -2.24 | 110.76      | 113.94   |
| 2   | T     | 301 | ADP  | N9-C8-N7 | -2.24 | 110.76      | 113.94   |
| 2   | H     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.77      | 113.94   |
| 2   | k     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.77      | 113.94   |
| 2   | U     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.77      | 113.94   |
| 2   | m     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.77      | 113.94   |
| 2   | Y     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.77      | 113.94   |
| 2   | E     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.77      | 113.94   |
| 2   | X     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.77      | 113.94   |
| 2   | f     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.77      | 113.94   |
| 2   | 7     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.77      | 113.94   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | c     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.77      | 113.94   |
| 2   | 3     | 301 | ADP  | C2-N1-C6 | 2.23  | 122.39      | 118.73   |
| 2   | O     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.77      | 113.94   |
| 2   | R     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.77      | 113.94   |
| 2   | I     | 301 | ADP  | C2-N1-C6 | 2.23  | 122.39      | 118.73   |
| 2   | F     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.77      | 113.94   |
| 2   | s     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.77      | 113.94   |
| 2   | b     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.78      | 113.94   |
| 2   | t     | 301 | ADP  | C2-N1-C6 | 2.23  | 122.39      | 118.73   |
| 2   | w     | 301 | ADP  | C2-N1-C6 | 2.23  | 122.39      | 118.73   |
| 2   | y     | 301 | ADP  | C2-N1-C6 | 2.23  | 122.39      | 118.73   |
| 2   | O     | 301 | ADP  | C2-N1-C6 | 2.23  | 122.39      | 118.73   |
| 2   | G     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.78      | 113.94   |
| 2   | D     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.78      | 113.94   |
| 2   | P     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.78      | 113.94   |
| 2   | j     | 301 | ADP  | N9-C8-N7 | -2.23 | 110.78      | 113.94   |
| 2   | Z     | 301 | ADP  | N9-C8-N7 | -2.22 | 110.78      | 113.94   |
| 2   | F     | 301 | ADP  | C2-N1-C6 | 2.22  | 122.38      | 118.73   |
| 2   | G     | 301 | ADP  | C2-N1-C6 | 2.22  | 122.38      | 118.73   |
| 2   | N     | 301 | ADP  | N9-C8-N7 | -2.22 | 110.78      | 113.94   |
| 2   | x     | 301 | ADP  | N9-C8-N7 | -2.22 | 110.78      | 113.94   |
| 2   | T     | 301 | ADP  | C2-N1-C6 | 2.22  | 122.38      | 118.73   |
| 2   | 6     | 301 | ADP  | N9-C8-N7 | -2.22 | 110.78      | 113.94   |
| 2   | y     | 301 | ADP  | N9-C8-N7 | -2.22 | 110.78      | 113.94   |
| 2   | J     | 301 | ADP  | N9-C8-N7 | -2.22 | 110.79      | 113.94   |
| 2   | W     | 301 | ADP  | N9-C8-N7 | -2.22 | 110.79      | 113.94   |
| 2   | a     | 301 | ADP  | N9-C8-N7 | -2.22 | 110.79      | 113.94   |
| 2   | U     | 301 | ADP  | C2-N1-C6 | 2.22  | 122.37      | 118.73   |
| 2   | c     | 301 | ADP  | C2-N1-C6 | 2.22  | 122.37      | 118.73   |
| 2   | Q     | 301 | ADP  | N9-C8-N7 | -2.22 | 110.79      | 113.94   |
| 2   | 1     | 301 | ADP  | C2-N1-C6 | 2.22  | 122.37      | 118.73   |
| 2   | C     | 301 | ADP  | C2-N1-C6 | 2.21  | 122.37      | 118.73   |
| 2   | b     | 301 | ADP  | C2-N1-C6 | 2.21  | 122.37      | 118.73   |
| 2   | 0     | 301 | ADP  | C2-N1-C6 | 2.21  | 122.36      | 118.73   |
| 2   | 5     | 301 | ADP  | N9-C8-N7 | -2.21 | 110.80      | 113.94   |
| 2   | i     | 301 | ADP  | C2-N1-C6 | 2.21  | 122.36      | 118.73   |
| 2   | f     | 301 | ADP  | C2-N1-C6 | 2.21  | 122.36      | 118.73   |
| 2   | 2     | 301 | ADP  | C2-N1-C6 | 2.21  | 122.36      | 118.73   |
| 2   | 5     | 301 | ADP  | C2-N1-C6 | 2.21  | 122.36      | 118.73   |
| 2   | R     | 301 | ADP  | C2-N1-C6 | 2.21  | 122.36      | 118.73   |
| 2   | C     | 301 | ADP  | N9-C8-N7 | -2.21 | 110.80      | 113.94   |
| 2   | 4     | 301 | ADP  | N9-C8-N7 | -2.21 | 110.80      | 113.94   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | I     | 301 | ADP  | N9-C8-N7 | -2.21 | 110.80      | 113.94   |
| 2   | n     | 301 | ADP  | N9-C8-N7 | -2.21 | 110.80      | 113.94   |
| 2   | j     | 301 | ADP  | C2-N1-C6 | 2.21  | 122.36      | 118.73   |
| 2   | 0     | 301 | ADP  | N9-C8-N7 | -2.21 | 110.81      | 113.94   |
| 2   | z     | 301 | ADP  | N9-C8-N7 | -2.21 | 110.81      | 113.94   |
| 2   | d     | 301 | ADP  | C2-N1-C6 | 2.21  | 122.36      | 118.73   |
| 2   | A     | 301 | ADP  | N9-C8-N7 | -2.21 | 110.81      | 113.94   |
| 2   | m     | 301 | ADP  | C2-N1-C6 | 2.21  | 122.35      | 118.73   |
| 2   | d     | 301 | ADP  | N9-C8-N7 | -2.21 | 110.81      | 113.94   |
| 2   | 4     | 301 | ADP  | C2-N1-C6 | 2.20  | 122.35      | 118.73   |
| 2   | V     | 301 | ADP  | C2-N1-C6 | 2.20  | 122.35      | 118.73   |
| 2   | B     | 301 | ADP  | C2-N1-C6 | 2.20  | 122.35      | 118.73   |
| 2   | J     | 301 | ADP  | C2-N1-C6 | 2.20  | 122.35      | 118.73   |
| 2   | 1     | 301 | ADP  | N9-C8-N7 | -2.20 | 110.81      | 113.94   |
| 2   | p     | 301 | ADP  | C2-N1-C6 | 2.20  | 122.35      | 118.73   |
| 2   | x     | 301 | ADP  | C2-N1-C6 | 2.20  | 122.35      | 118.73   |
| 2   | e     | 301 | ADP  | C2-N1-C6 | 2.20  | 122.34      | 118.73   |
| 2   | 6     | 301 | ADP  | C2-N1-C6 | 2.20  | 122.34      | 118.73   |
| 2   | K     | 301 | ADP  | C2-N1-C6 | 2.20  | 122.34      | 118.73   |
| 2   | 2     | 301 | ADP  | N9-C8-N7 | -2.20 | 110.82      | 113.94   |
| 2   | K     | 301 | ADP  | N9-C8-N7 | -2.20 | 110.82      | 113.94   |
| 2   | N     | 301 | ADP  | C2-N1-C6 | 2.20  | 122.34      | 118.73   |
| 2   | Q     | 301 | ADP  | C2-N1-C6 | 2.20  | 122.34      | 118.73   |
| 2   | W     | 301 | ADP  | C2-N1-C6 | 2.20  | 122.34      | 118.73   |
| 2   | h     | 301 | ADP  | C2-N1-C6 | 2.20  | 122.34      | 118.73   |
| 2   | D     | 301 | ADP  | C2-N1-C6 | 2.20  | 122.34      | 118.73   |
| 2   | z     | 301 | ADP  | C2-N1-C6 | 2.20  | 122.34      | 118.73   |
| 2   | h     | 301 | ADP  | N9-C8-N7 | -2.20 | 110.82      | 113.94   |
| 2   | i     | 301 | ADP  | N9-C8-N7 | -2.20 | 110.82      | 113.94   |
| 2   | E     | 301 | ADP  | C2-N1-C6 | 2.20  | 122.34      | 118.73   |
| 2   | M     | 301 | ADP  | C2-N1-C6 | 2.20  | 122.34      | 118.73   |
| 2   | V     | 301 | ADP  | N9-C8-N7 | -2.19 | 110.83      | 113.94   |
| 2   | L     | 301 | ADP  | C2-N1-C6 | 2.19  | 122.33      | 118.73   |
| 2   | X     | 301 | ADP  | C2-N1-C6 | 2.19  | 122.33      | 118.73   |
| 2   | g     | 301 | ADP  | C2-N1-C6 | 2.19  | 122.33      | 118.73   |
| 2   | A     | 301 | ADP  | C2-N1-C6 | 2.19  | 122.33      | 118.73   |
| 2   | a     | 301 | ADP  | C2-N1-C6 | 2.19  | 122.33      | 118.73   |
| 2   | n     | 301 | ADP  | C2-N1-C6 | 2.19  | 122.33      | 118.73   |
| 2   | q     | 301 | ADP  | C2-N1-C6 | 2.19  | 122.32      | 118.73   |
| 2   | H     | 301 | ADP  | C2-N1-C6 | 2.19  | 122.32      | 118.73   |
| 2   | o     | 301 | ADP  | C2-N1-C6 | 2.19  | 122.32      | 118.73   |
| 2   | v     | 301 | ADP  | C2-N1-C6 | 2.19  | 122.32      | 118.73   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | l     | 301 | ADP  | C2-N1-C6 | 2.19  | 122.32      | 118.73   |
| 2   | Y     | 301 | ADP  | C2-N1-C6 | 2.18  | 122.31      | 118.73   |
| 2   | s     | 301 | ADP  | C2-N1-C6 | 2.18  | 122.31      | 118.73   |
| 2   | S     | 301 | ADP  | C2-N1-C6 | 2.18  | 122.31      | 118.73   |
| 2   | u     | 301 | ADP  | C2-N1-C6 | 2.18  | 122.31      | 118.73   |
| 2   | v     | 301 | ADP  | N9-C8-N7 | -2.18 | 110.84      | 113.94   |
| 2   | P     | 301 | ADP  | C2-N1-C6 | 2.18  | 122.31      | 118.73   |
| 2   | 7     | 301 | ADP  | C2-N1-C6 | 2.18  | 122.31      | 118.73   |
| 2   | Z     | 301 | ADP  | C2-N1-C6 | 2.18  | 122.30      | 118.73   |
| 2   | r     | 301 | ADP  | C2-N1-C6 | 2.17  | 122.29      | 118.73   |
| 2   | k     | 301 | ADP  | C2-N1-C6 | 2.16  | 122.28      | 118.73   |

There are no chirality outliers.

All (480) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | 0     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | 0     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | 1     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | 1     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | 2     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | 2     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | 3     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | 3     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | 4     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | 4     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | 5     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | 5     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | 6     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | 6     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | 7     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | 7     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | A     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | A     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | B     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | B     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | C     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | C     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | D     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | D     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | E     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | E     | 301 | ADP  | C2'-C1'-N9-C8  |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | F     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | F     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | G     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | G     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | H     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | H     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | I     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | I     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | J     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | J     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | K     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | K     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | L     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | L     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | M     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | M     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | N     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | N     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | O     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | O     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | P     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | P     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | Q     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | Q     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | R     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | R     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | S     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | S     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | T     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | T     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | U     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | U     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | V     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | V     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | W     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | W     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | X     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | X     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | Y     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | Y     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | Z     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | Z     | 301 | ADP  | C2'-C1'-N9-C8  |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | a     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | a     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | b     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | b     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | c     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | c     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | d     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | d     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | e     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | e     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | f     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | f     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | g     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | g     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | h     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | h     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | i     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | i     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | j     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | j     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | k     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | k     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | l     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | l     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | m     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | m     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | n     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | n     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | o     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | o     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | p     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | p     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | q     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | q     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | r     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | r     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | s     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | s     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | t     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | t     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | u     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | u     | 301 | ADP  | C2'-C1'-N9-C8  |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | v     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | v     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | w     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | w     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | x     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | x     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | y     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | y     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | z     | 301 | ADP  | C5'-O5'-PA-O2A |
| 2   | z     | 301 | ADP  | C2'-C1'-N9-C8  |
| 2   | 0     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | 1     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | 2     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | 3     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | 4     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | 5     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | 6     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | 7     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | A     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | B     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | C     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | D     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | E     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | F     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | G     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | H     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | I     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | J     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | K     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | L     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | M     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | N     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | O     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | P     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | Q     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | R     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | S     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | T     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | U     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | V     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | W     | 301 | ADP  | C2'-C1'-N9-C4  |
| 2   | X     | 301 | ADP  | C2'-C1'-N9-C4  |

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| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 2   | Y     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | Z     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | a     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | b     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | c     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | d     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | e     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | f     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | g     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | h     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | i     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | j     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | k     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | l     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | m     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | n     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | o     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | p     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | q     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | r     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | s     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | t     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | u     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | v     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | w     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | x     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | y     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | z     | 301 | ADP  | C2'-C1'-N9-C4 |
| 2   | 0     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | 1     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | 2     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | 3     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | 4     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | 5     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | 6     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | 7     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | A     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | B     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | C     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | D     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | E     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | F     | 301 | ADP  | PB-O3A-PA-O2A |

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| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 2   | G     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | H     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | I     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | J     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | K     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | L     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | M     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | N     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | O     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | P     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | Q     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | R     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | S     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | T     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | U     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | V     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | W     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | X     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | Y     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | Z     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | a     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | b     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | c     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | d     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | e     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | f     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | g     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | h     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | i     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | j     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | k     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | l     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | m     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | n     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | o     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | p     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | q     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | r     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | s     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | t     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | u     | 301 | ADP  | PB-O3A-PA-O2A |
| 2   | v     | 301 | ADP  | PB-O3A-PA-O2A |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | w     | 301 | ADP  | PB-O3A-PA-O2A  |
| 2   | x     | 301 | ADP  | PB-O3A-PA-O2A  |
| 2   | y     | 301 | ADP  | PB-O3A-PA-O2A  |
| 2   | z     | 301 | ADP  | PB-O3A-PA-O2A  |
| 2   | 0     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | 0     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | 1     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | 1     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | 2     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | 2     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | 3     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | 3     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | 4     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | 4     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | 5     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | 5     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | 6     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | 6     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | 7     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | 7     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | A     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | A     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | B     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | B     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | C     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | C     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | D     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | D     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | E     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | E     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | F     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | F     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | G     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | G     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | H     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | H     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | I     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | I     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | J     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | J     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | K     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | K     | 301 | ADP  | C5'-O5'-PA-O3A |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | L     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | L     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | M     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | M     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | N     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | N     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | O     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | O     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | P     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | P     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | Q     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | Q     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | R     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | R     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | S     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | S     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | T     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | T     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | U     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | U     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | V     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | V     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | W     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | W     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | X     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | X     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | Y     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | Y     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | Z     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | Z     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | a     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | a     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | b     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | b     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | c     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | c     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | d     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | d     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | e     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | e     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | f     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | f     | 301 | ADP  | C5'-O5'-PA-O3A |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | g     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | g     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | h     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | h     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | i     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | i     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | j     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | j     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | k     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | k     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | l     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | l     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | m     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | m     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | n     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | n     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | o     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | o     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | p     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | p     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | q     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | q     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | r     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | r     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | s     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | s     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | t     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | t     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | u     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | u     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | v     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | v     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | w     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | w     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | x     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | x     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | y     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | y     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | z     | 301 | ADP  | C5'-O5'-PA-O1A |
| 2   | z     | 301 | ADP  | C5'-O5'-PA-O3A |
| 2   | 0     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | 1     | 301 | ADP  | C4'-C5'-O5'-PA |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | 2     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | 3     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | 4     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | 5     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | 6     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | 7     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | A     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | B     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | C     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | D     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | E     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | F     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | G     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | H     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | I     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | J     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | K     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | L     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | M     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | N     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | O     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | P     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | Q     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | R     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | S     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | T     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | U     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | V     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | W     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | X     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | Y     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | Z     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | a     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | b     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | c     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | d     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | e     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | f     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | g     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | h     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | i     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | j     | 301 | ADP  | C4'-C5'-O5'-PA |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | k     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | l     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | m     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | n     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | o     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | p     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | q     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | r     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | s     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | t     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | u     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | v     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | w     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | x     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | y     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | z     | 301 | ADP  | C4'-C5'-O5'-PA |
| 2   | 0     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | 1     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | 2     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | 3     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | 4     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | 5     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | 6     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | 7     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | A     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | B     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | C     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | D     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | E     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | F     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | G     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | H     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | I     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | J     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | K     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | L     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | M     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | N     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | O     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | P     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | Q     | 301 | ADP  | PB-O3A-PA-O1A  |
| 2   | R     | 301 | ADP  | PB-O3A-PA-O1A  |

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| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 2   | S     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | T     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | U     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | V     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | W     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | X     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | Y     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | Z     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | a     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | b     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | c     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | d     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | e     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | f     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | g     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | h     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | i     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | j     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | k     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | l     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | m     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | n     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | o     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | p     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | q     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | r     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | s     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | t     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | u     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | v     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | w     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | x     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | y     | 301 | ADP  | PB-O3A-PA-O1A |
| 2   | z     | 301 | ADP  | PB-O3A-PA-O1A |

There are no ring outliers.

60 monomers are involved in 120 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | w     | 301 | ADP  | 2       | 0            |
| 2   | i     | 301 | ADP  | 2       | 0            |
| 2   | Y     | 301 | ADP  | 2       | 0            |

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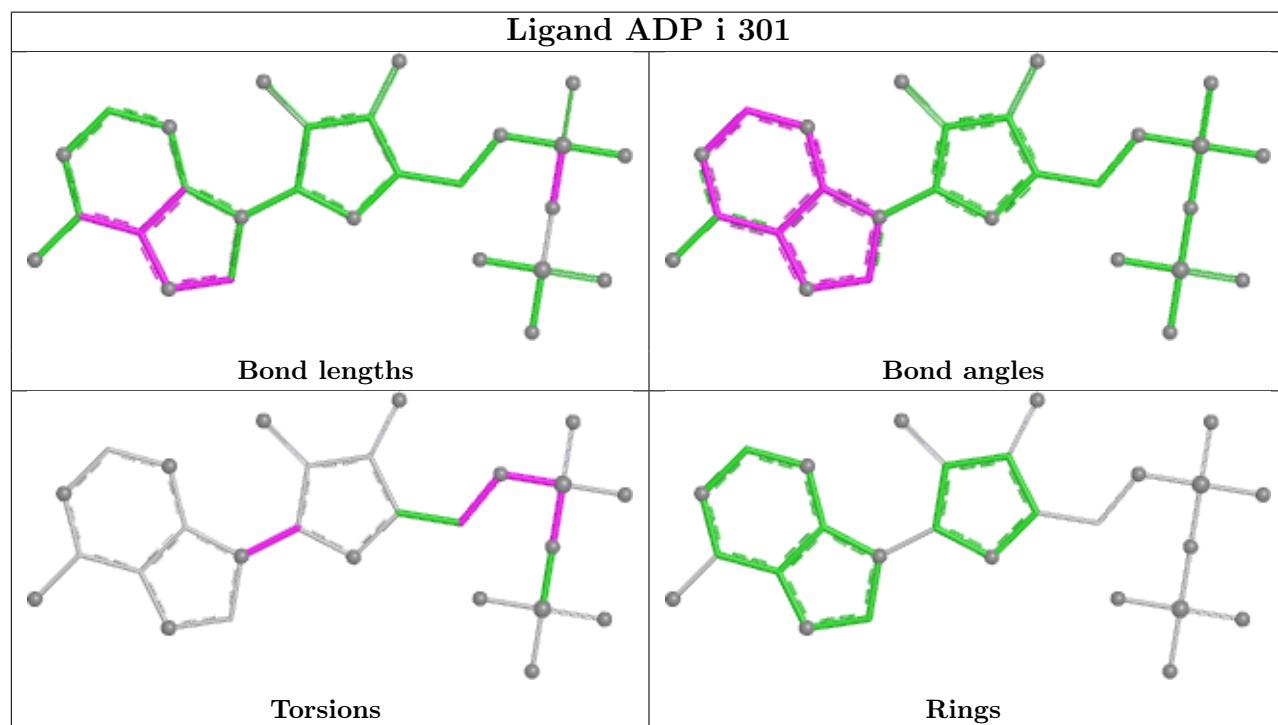
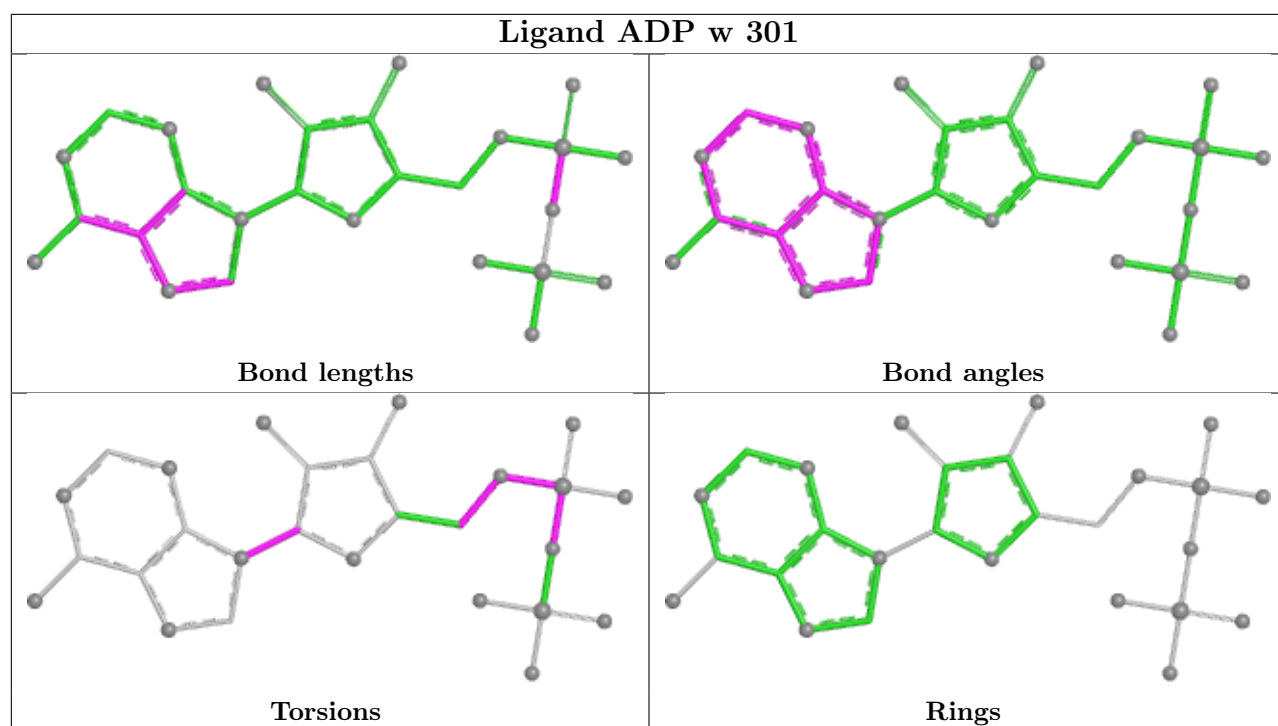
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | E     | 301 | ADP  | 2       | 0            |
| 2   | P     | 301 | ADP  | 2       | 0            |
| 2   | f     | 301 | ADP  | 2       | 0            |
| 2   | r     | 301 | ADP  | 2       | 0            |
| 2   | M     | 301 | ADP  | 2       | 0            |
| 2   | n     | 301 | ADP  | 2       | 0            |
| 2   | t     | 301 | ADP  | 2       | 0            |
| 2   | O     | 301 | ADP  | 2       | 0            |
| 2   | e     | 301 | ADP  | 2       | 0            |
| 2   | H     | 301 | ADP  | 2       | 0            |
| 2   | 3     | 301 | ADP  | 2       | 0            |
| 2   | U     | 301 | ADP  | 2       | 0            |
| 2   | J     | 301 | ADP  | 2       | 0            |
| 2   | u     | 301 | ADP  | 2       | 0            |
| 2   | S     | 301 | ADP  | 2       | 0            |
| 2   | s     | 301 | ADP  | 2       | 0            |
| 2   | 2     | 301 | ADP  | 2       | 0            |
| 2   | z     | 301 | ADP  | 2       | 0            |
| 2   | 7     | 301 | ADP  | 2       | 0            |
| 2   | m     | 301 | ADP  | 2       | 0            |
| 2   | V     | 301 | ADP  | 2       | 0            |
| 2   | D     | 301 | ADP  | 2       | 0            |
| 2   | X     | 301 | ADP  | 2       | 0            |
| 2   | G     | 301 | ADP  | 2       | 0            |
| 2   | o     | 301 | ADP  | 2       | 0            |
| 2   | L     | 301 | ADP  | 2       | 0            |
| 2   | T     | 301 | ADP  | 2       | 0            |
| 2   | 5     | 301 | ADP  | 2       | 0            |
| 2   | B     | 301 | ADP  | 2       | 0            |
| 2   | v     | 301 | ADP  | 2       | 0            |
| 2   | F     | 301 | ADP  | 2       | 0            |
| 2   | C     | 301 | ADP  | 2       | 0            |
| 2   | g     | 301 | ADP  | 2       | 0            |
| 2   | a     | 301 | ADP  | 2       | 0            |
| 2   | W     | 301 | ADP  | 2       | 0            |
| 2   | j     | 301 | ADP  | 2       | 0            |
| 2   | 4     | 301 | ADP  | 2       | 0            |
| 2   | q     | 301 | ADP  | 2       | 0            |
| 2   | d     | 301 | ADP  | 2       | 0            |
| 2   | y     | 301 | ADP  | 2       | 0            |
| 2   | I     | 301 | ADP  | 2       | 0            |
| 2   | Q     | 301 | ADP  | 2       | 0            |

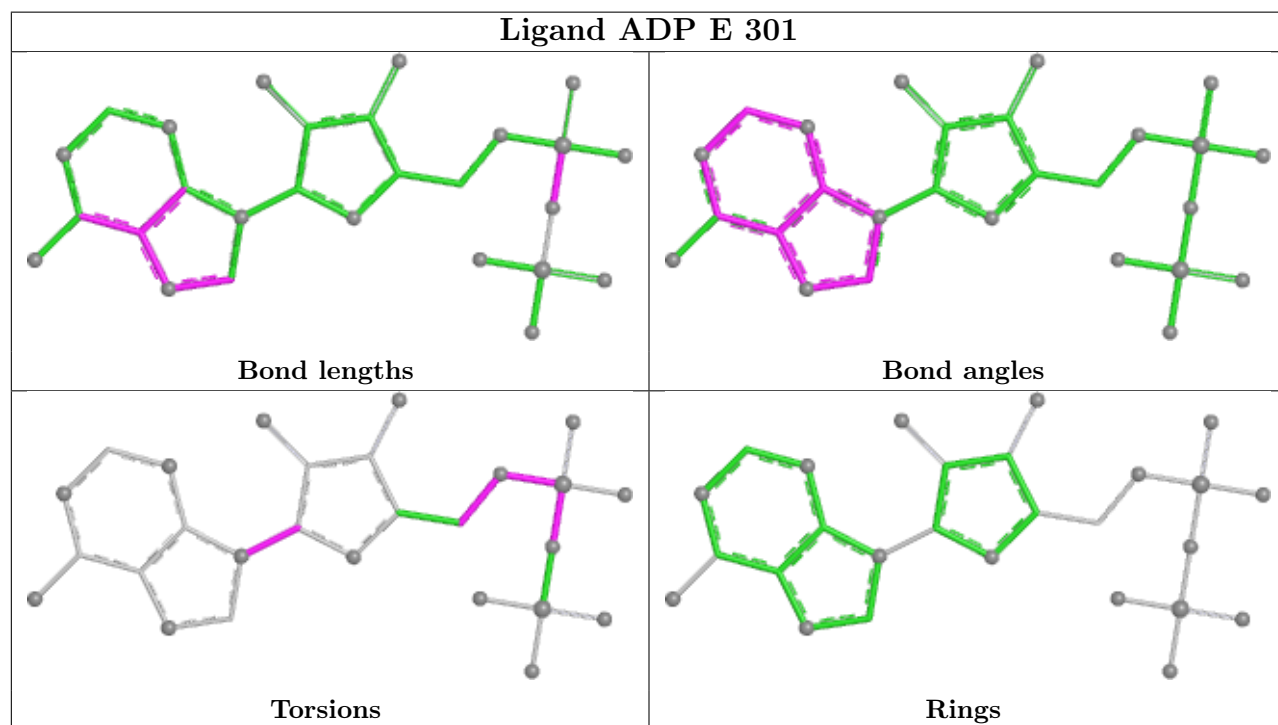
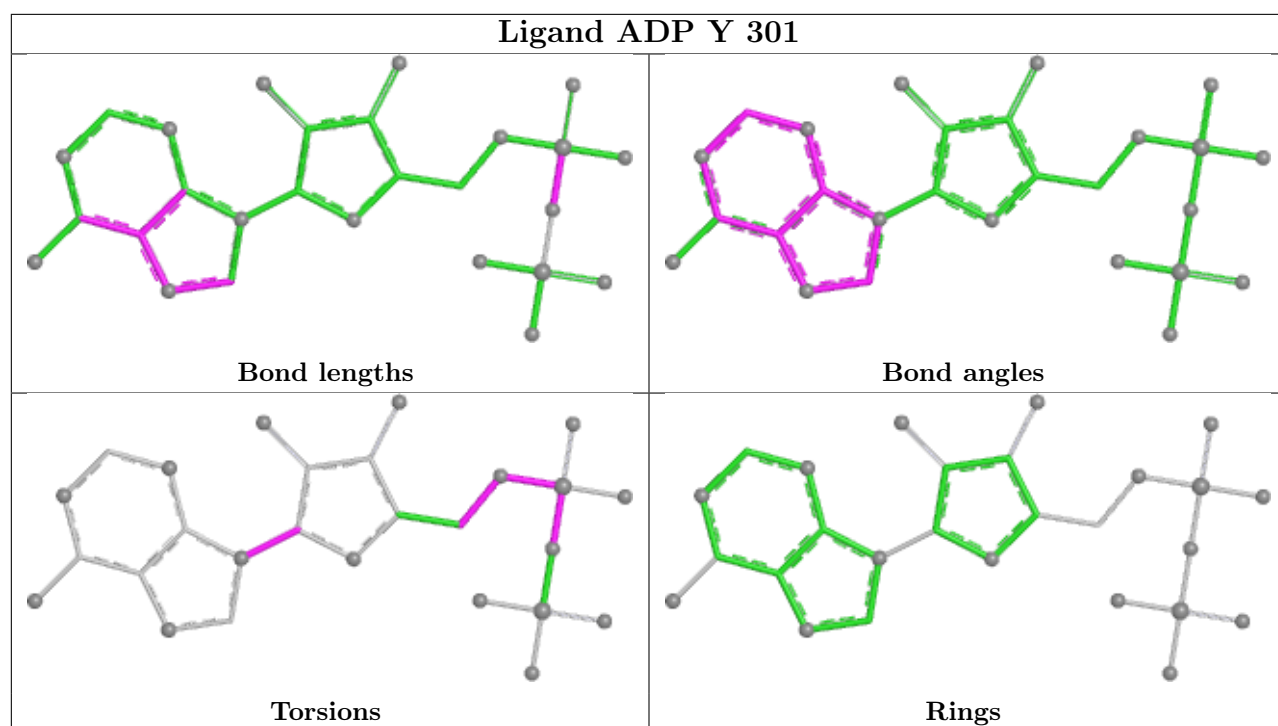
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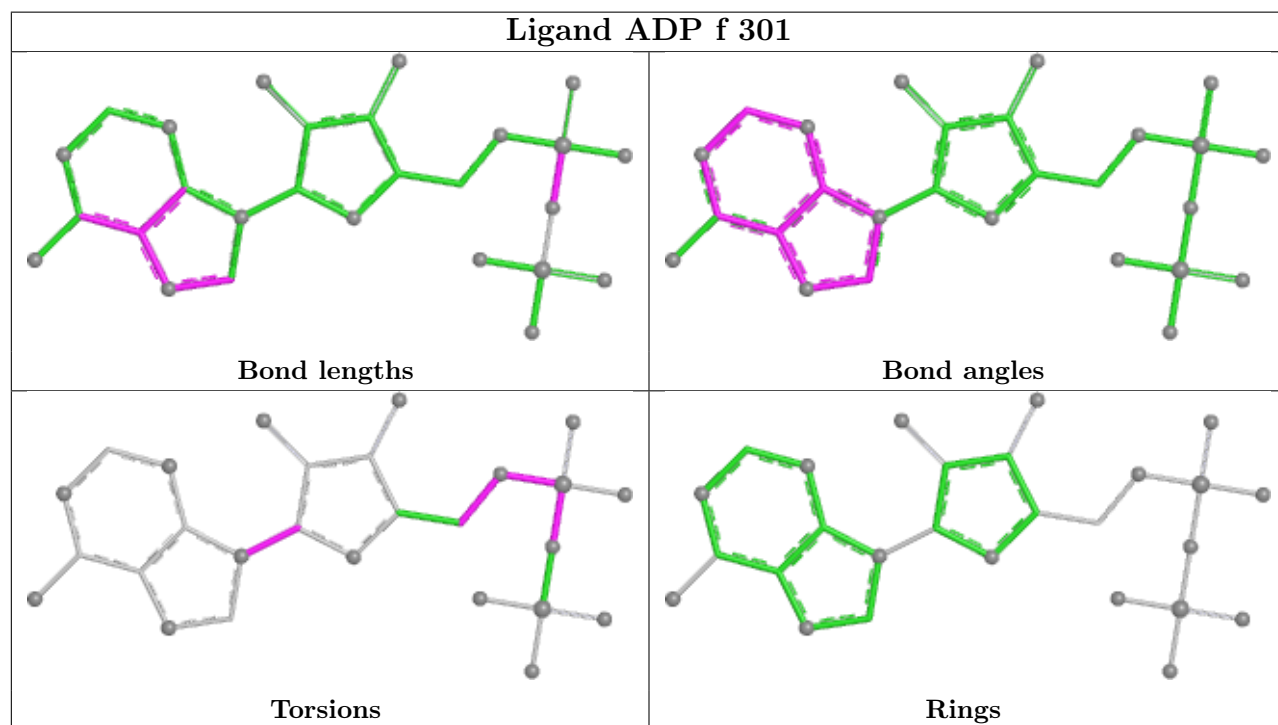
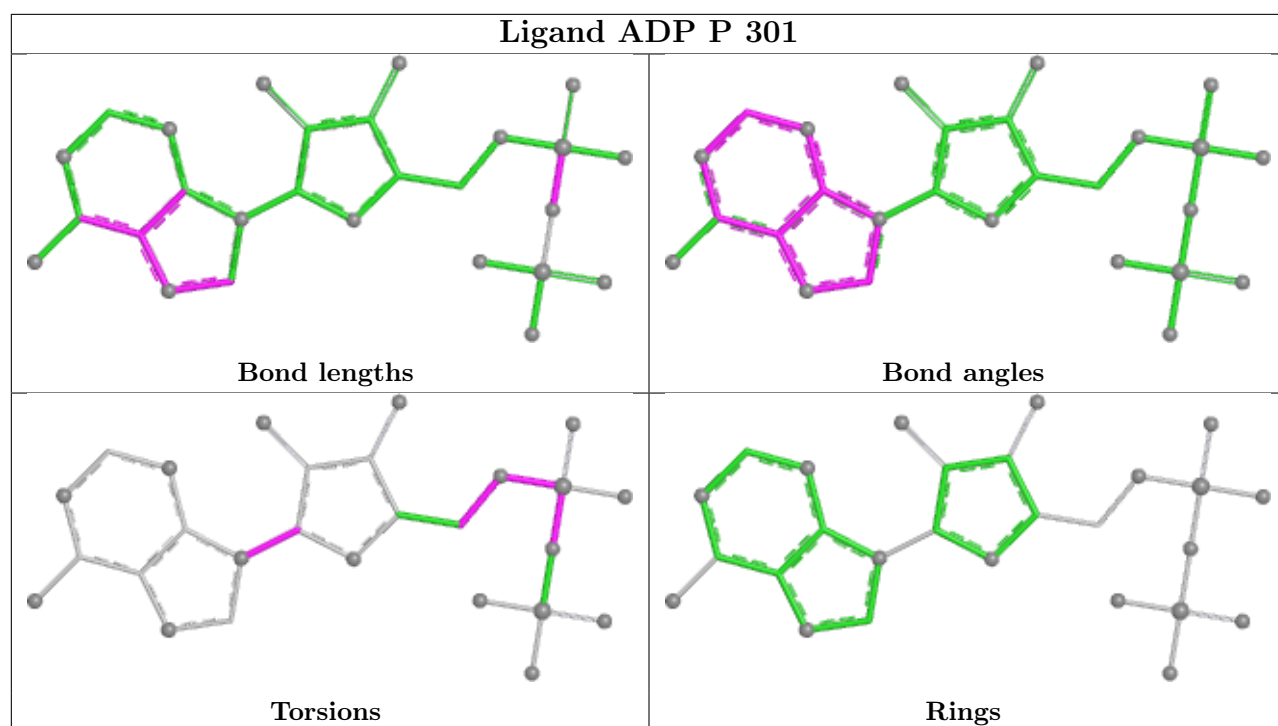
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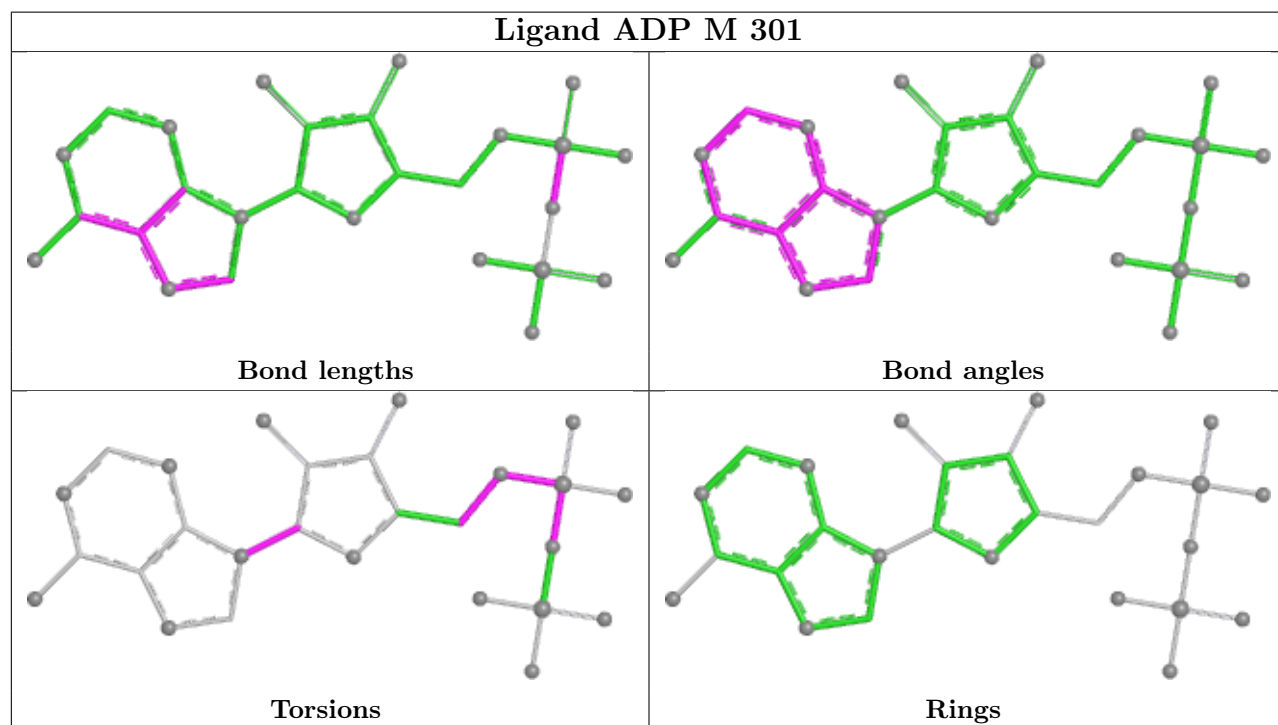
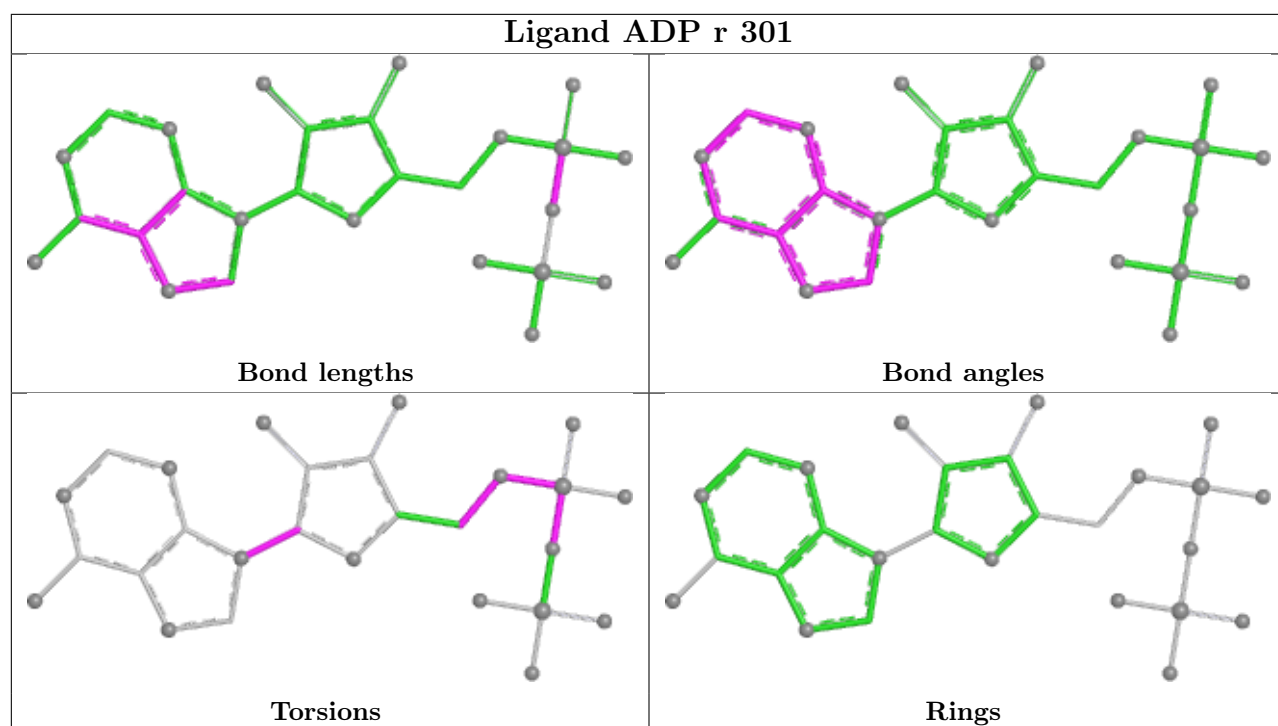
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | 1     | 301 | ADP  | 2       | 0            |
| 2   | k     | 301 | ADP  | 2       | 0            |
| 2   | x     | 301 | ADP  | 2       | 0            |
| 2   | b     | 301 | ADP  | 2       | 0            |
| 2   | l     | 301 | ADP  | 2       | 0            |
| 2   | h     | 301 | ADP  | 2       | 0            |
| 2   | K     | 301 | ADP  | 2       | 0            |
| 2   | R     | 301 | ADP  | 2       | 0            |
| 2   | 0     | 301 | ADP  | 2       | 0            |
| 2   | Z     | 301 | ADP  | 2       | 0            |
| 2   | c     | 301 | ADP  | 2       | 0            |
| 2   | 6     | 301 | ADP  | 2       | 0            |
| 2   | N     | 301 | ADP  | 2       | 0            |
| 2   | p     | 301 | ADP  | 2       | 0            |
| 2   | A     | 301 | ADP  | 2       | 0            |

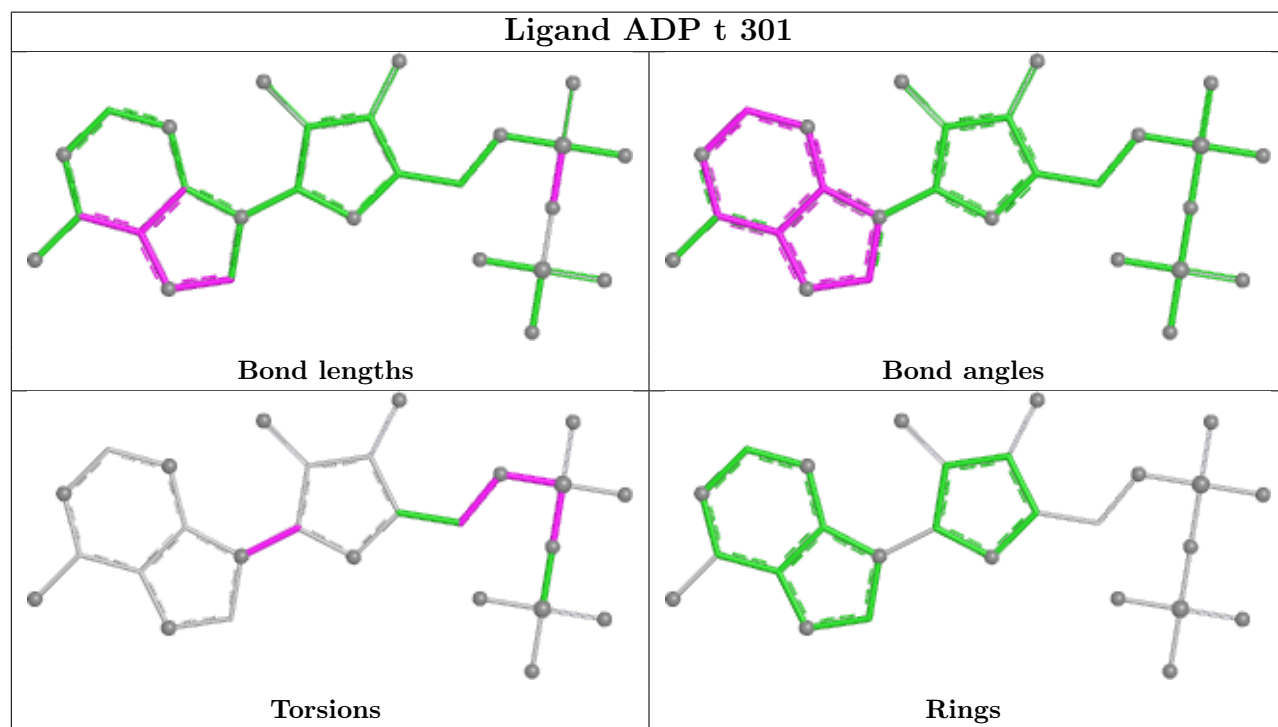
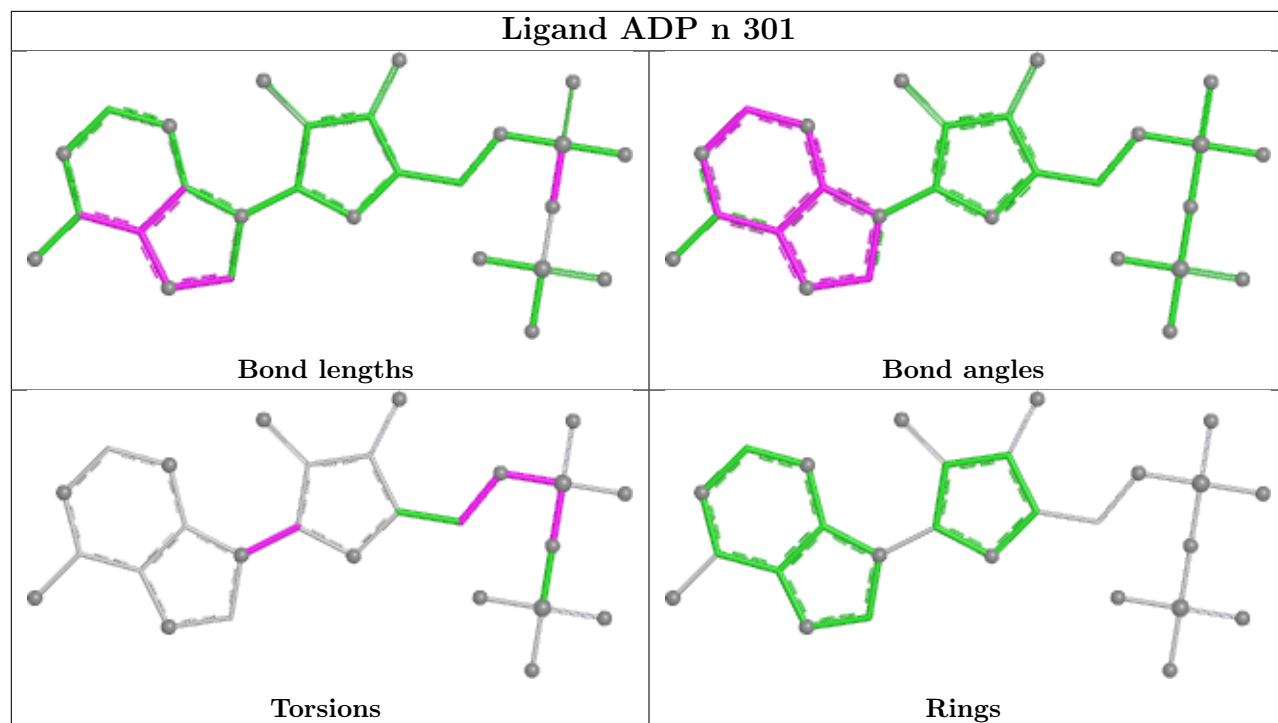
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

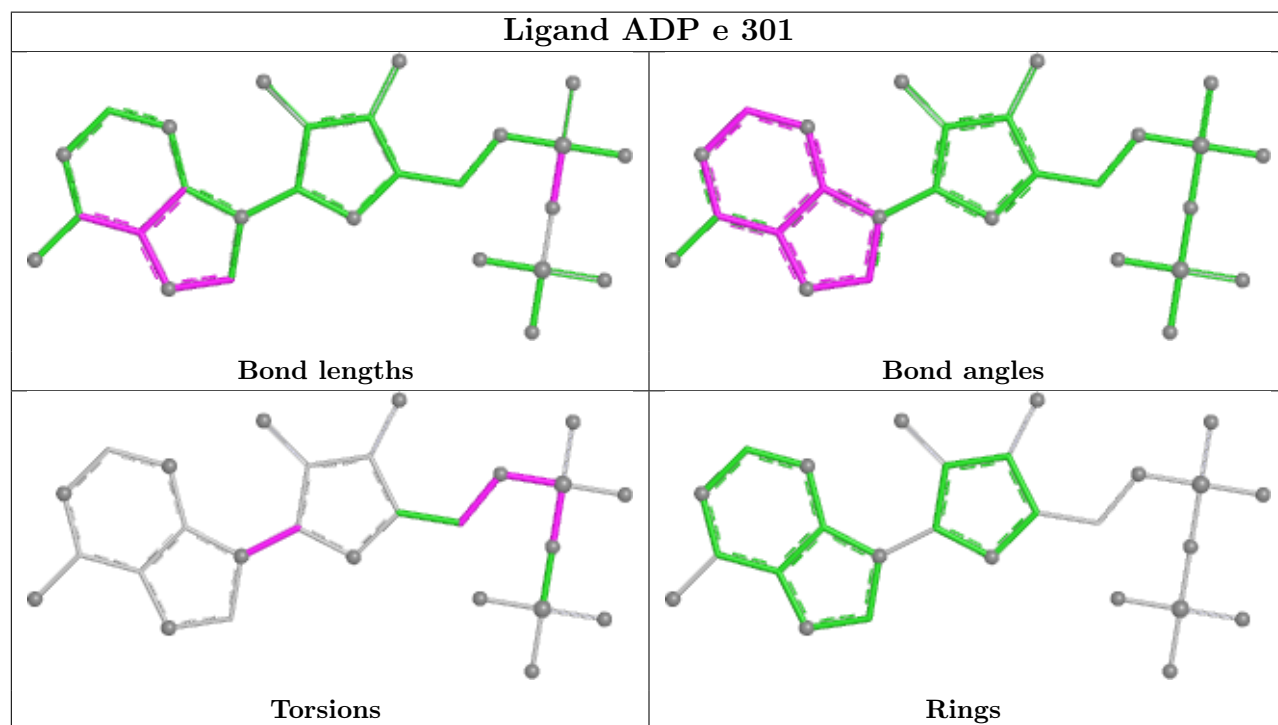
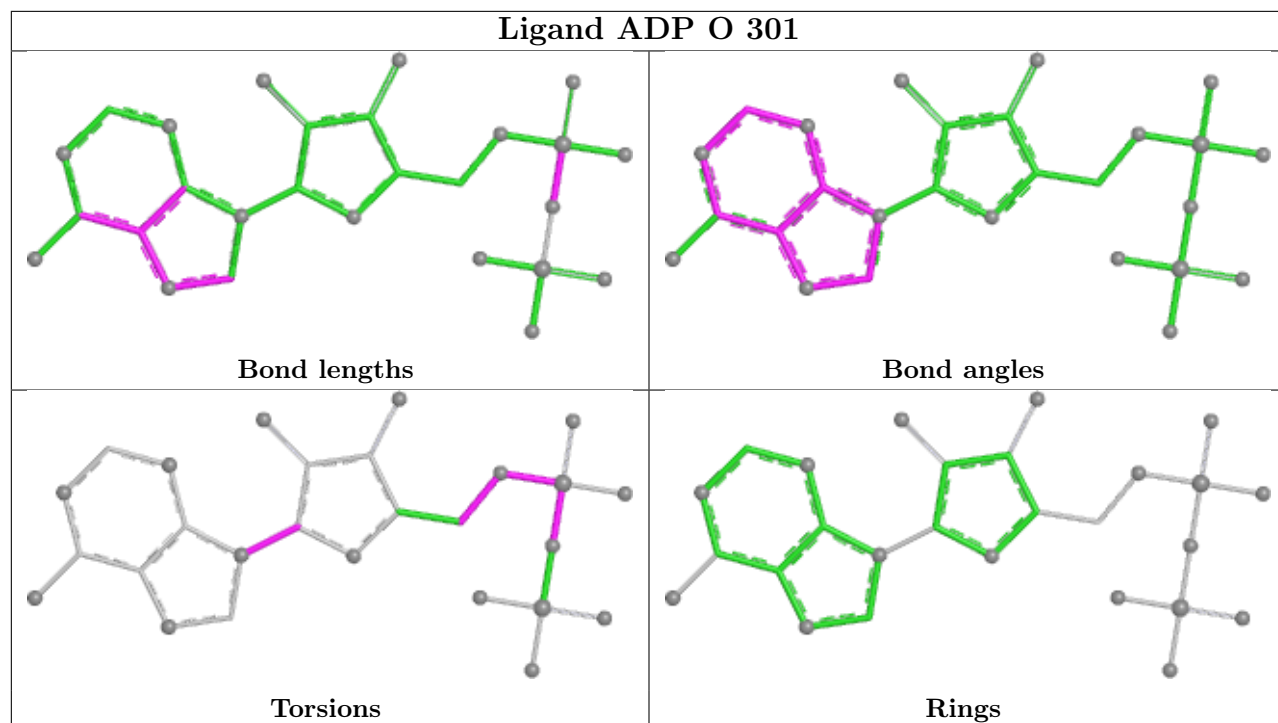


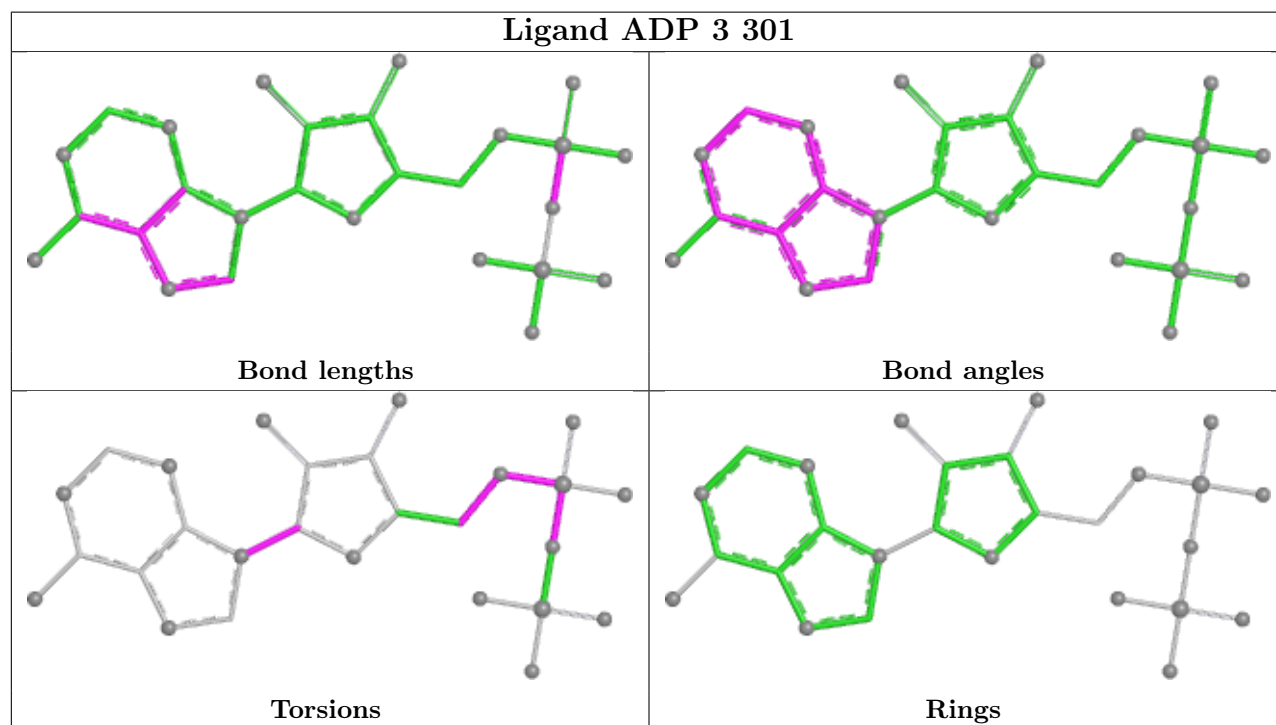
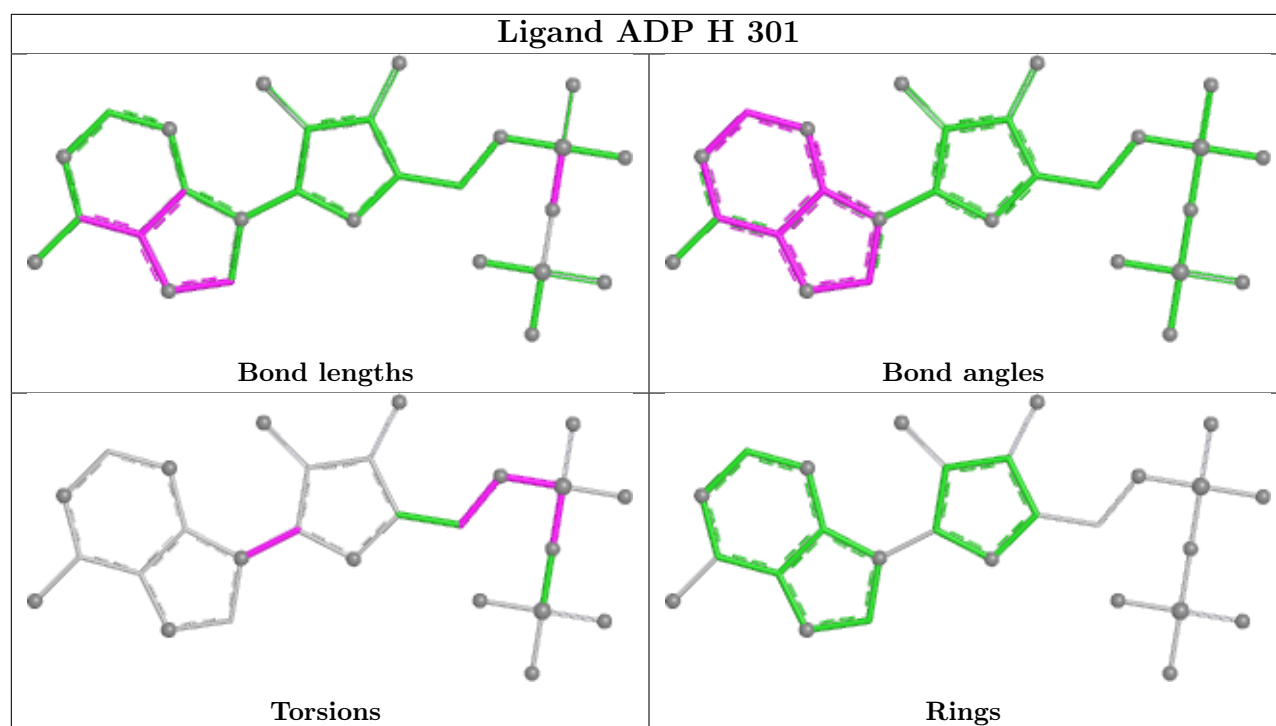


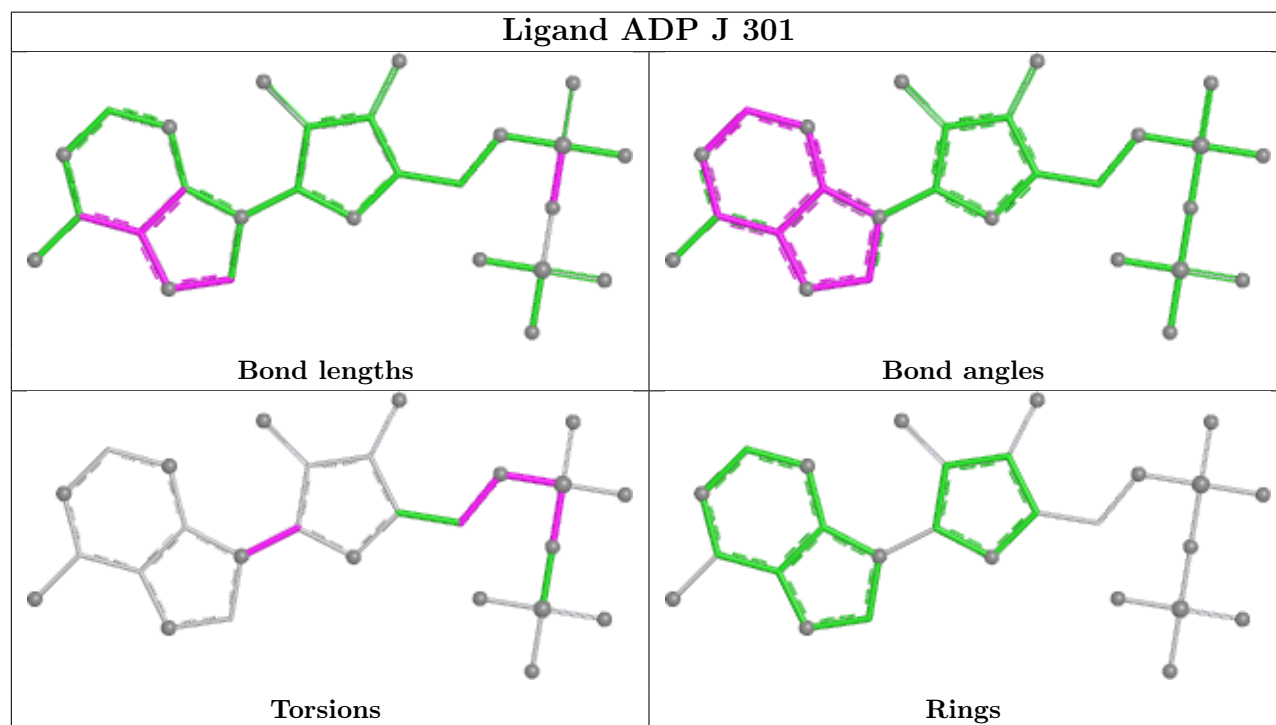
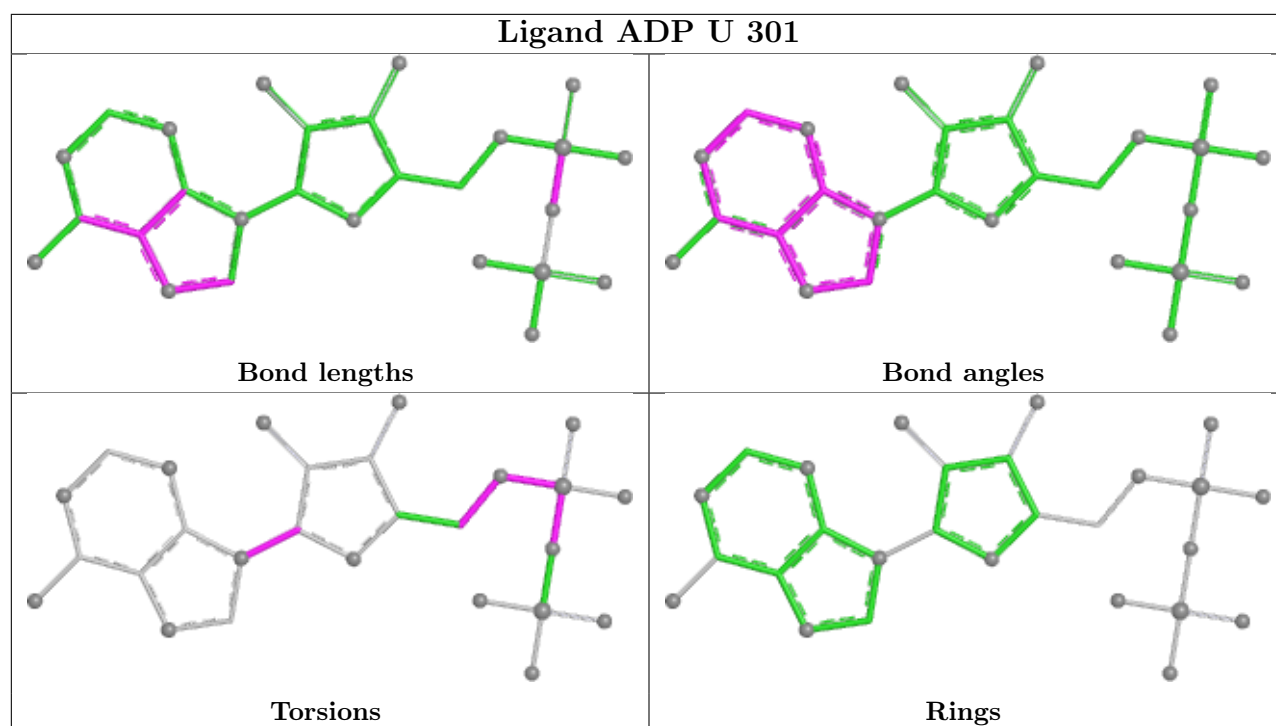


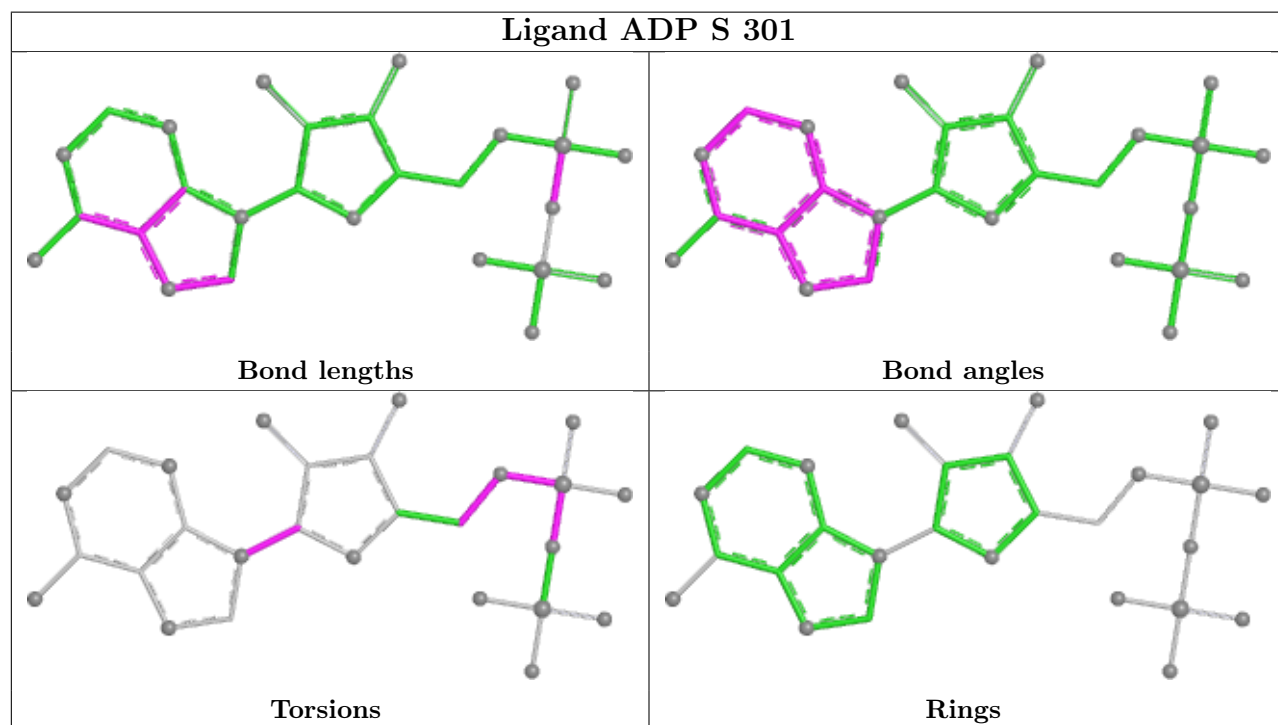
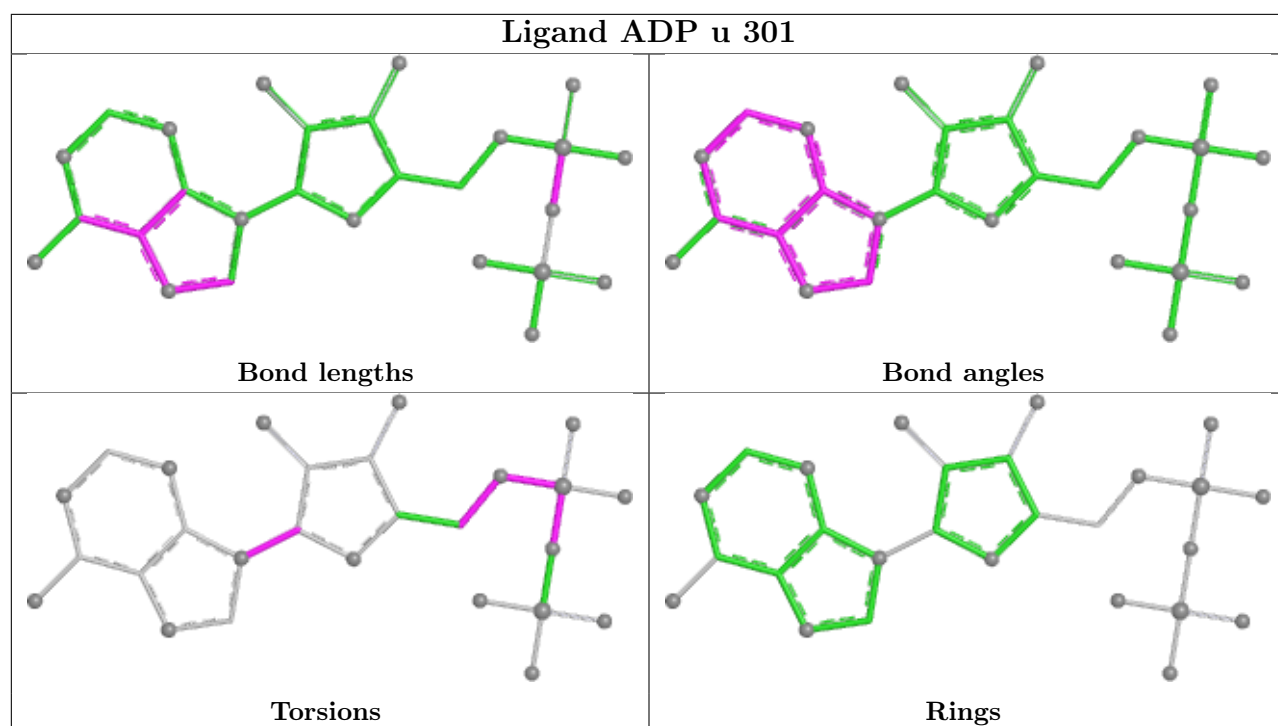


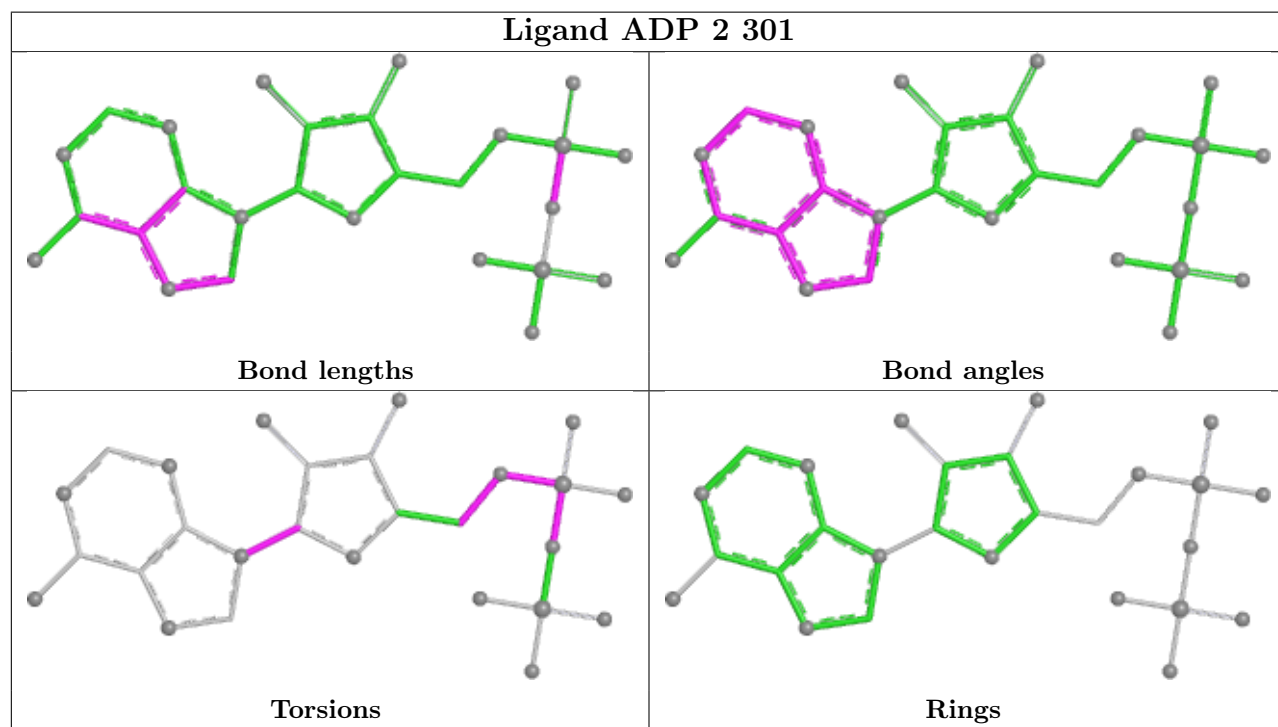
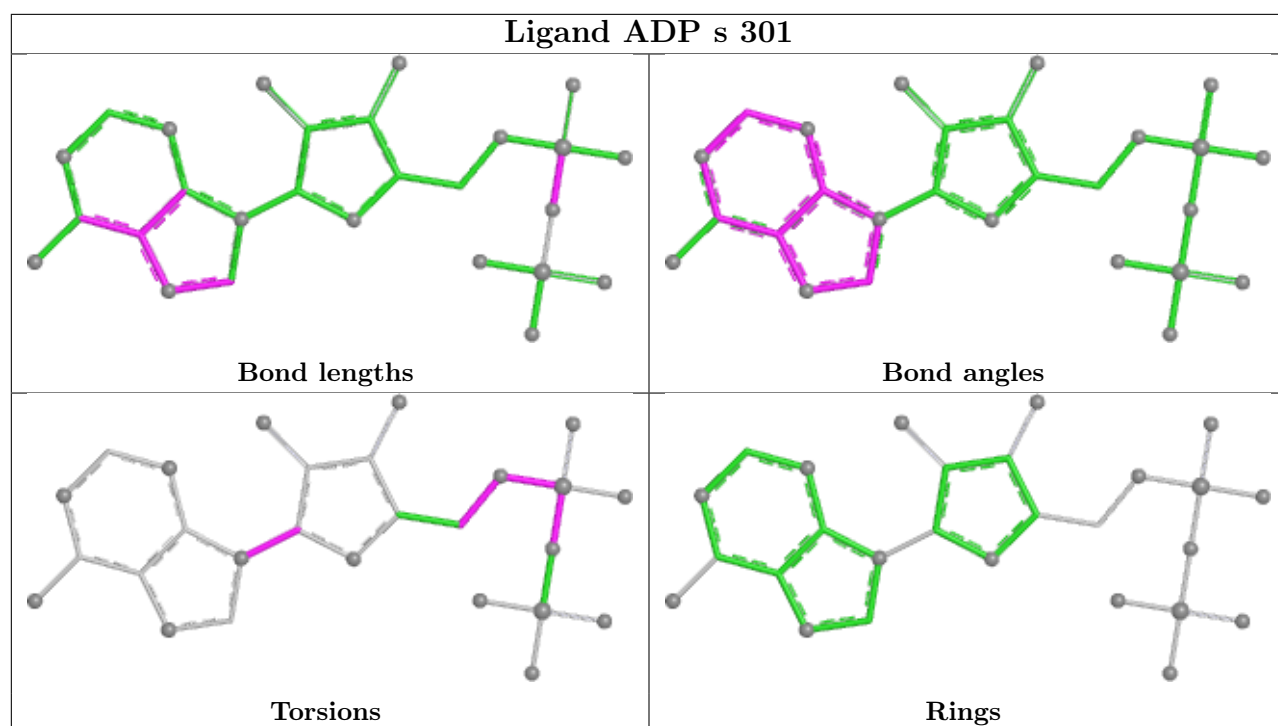


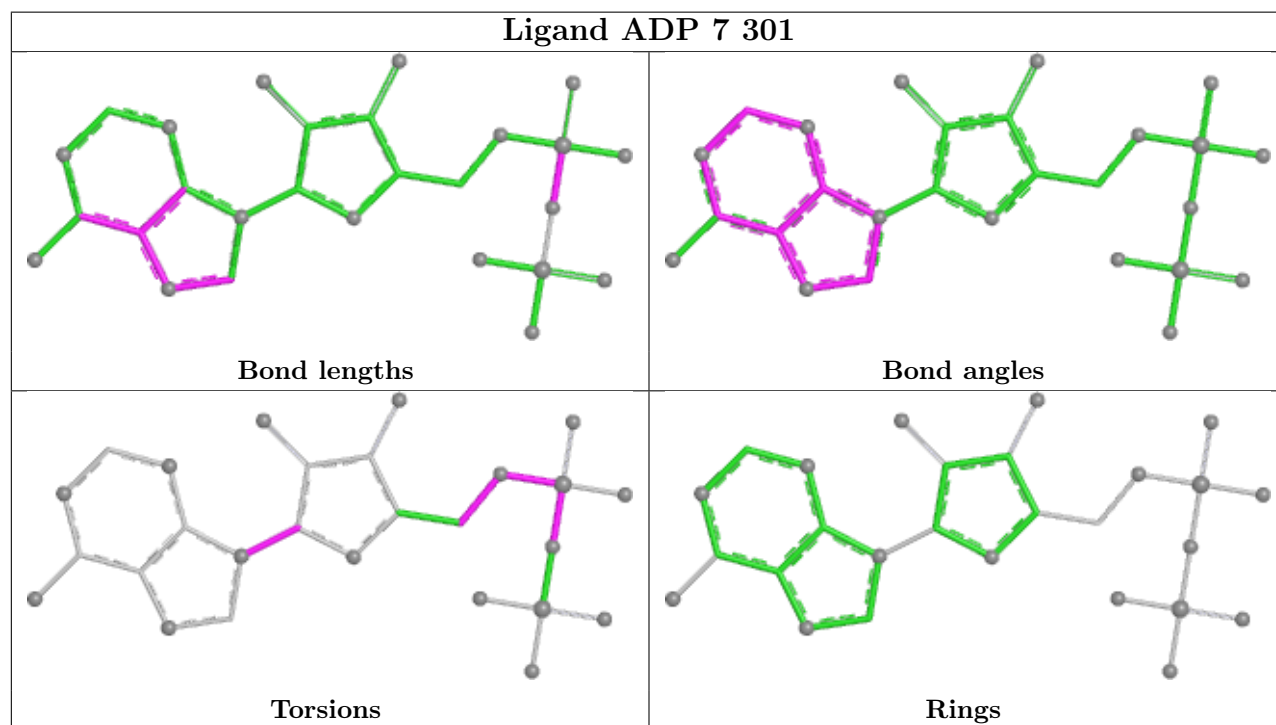
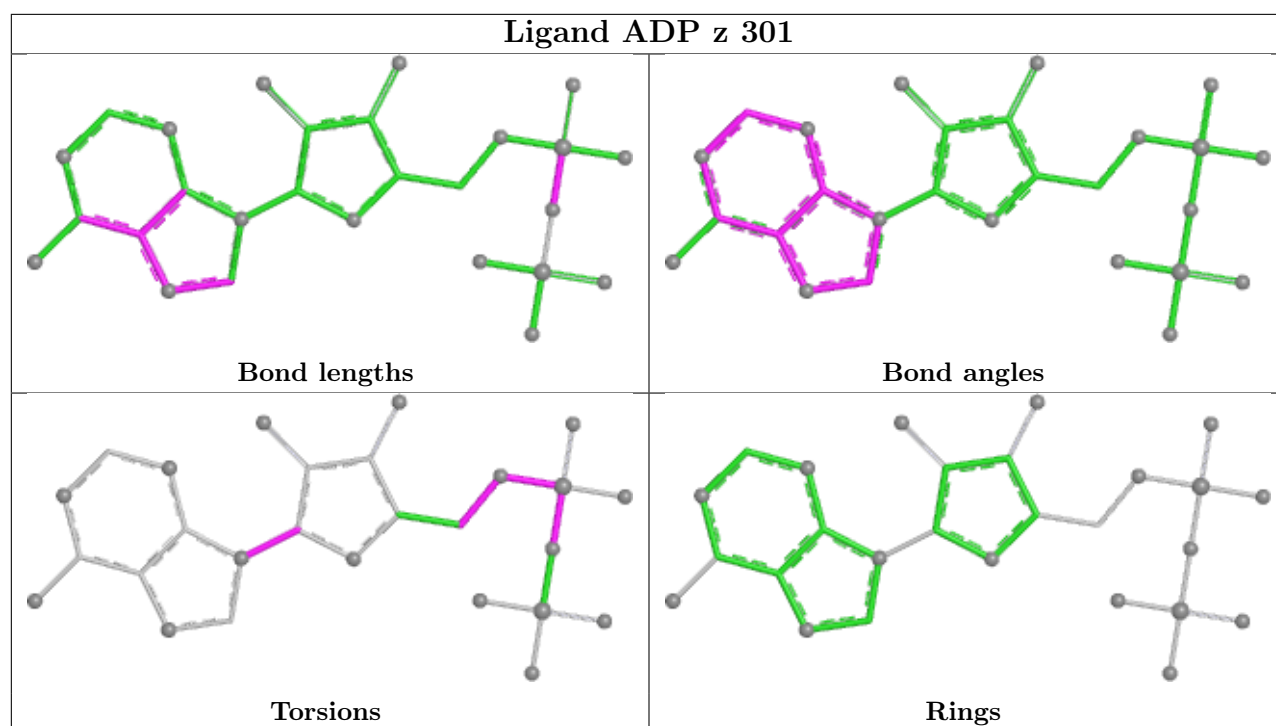


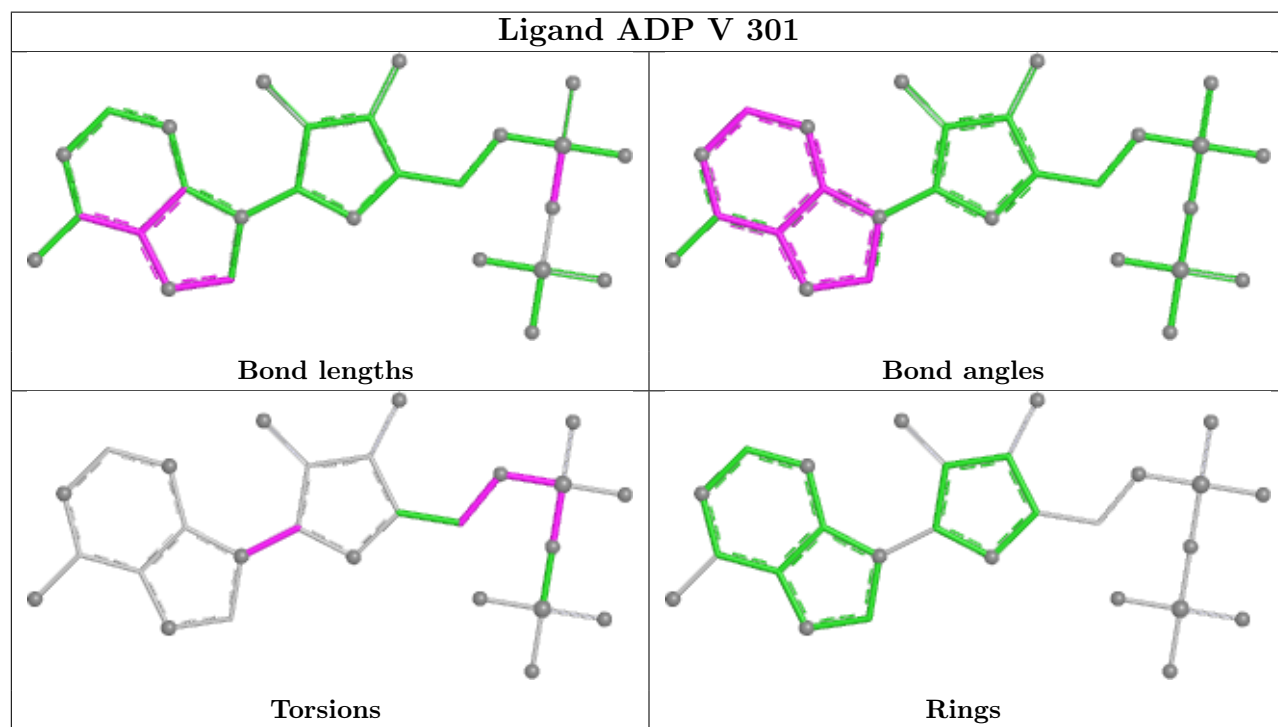
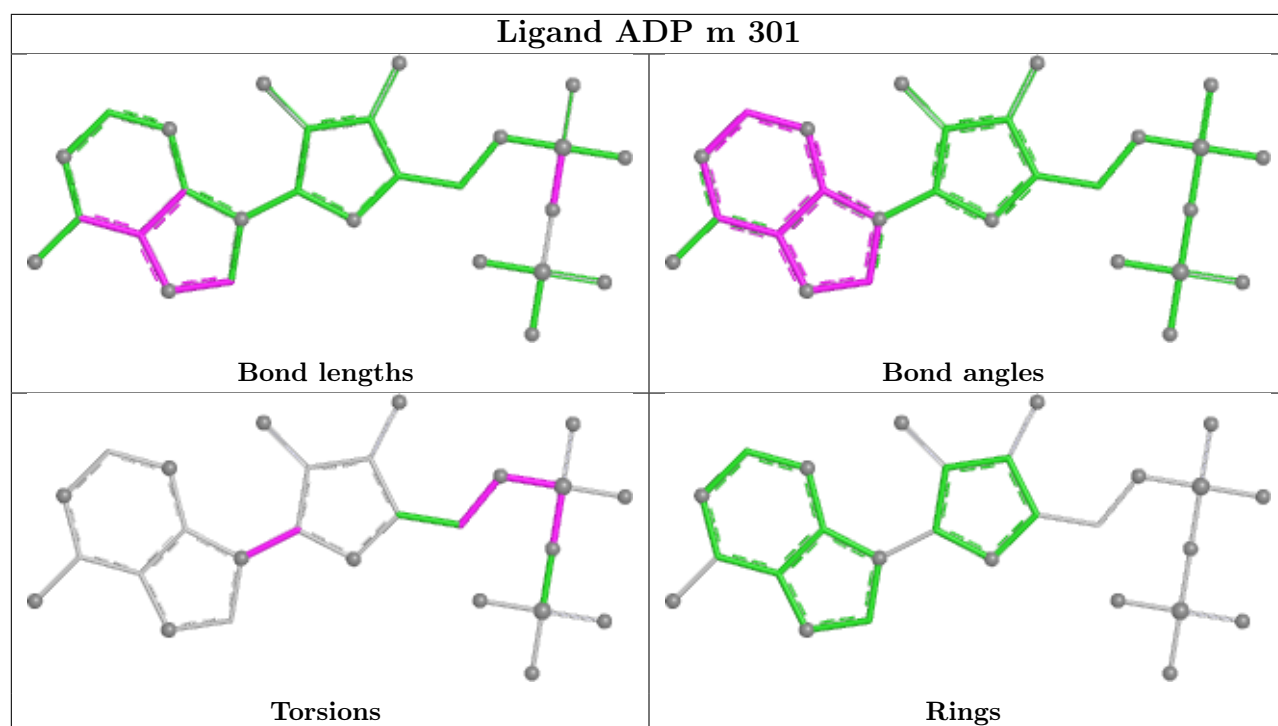


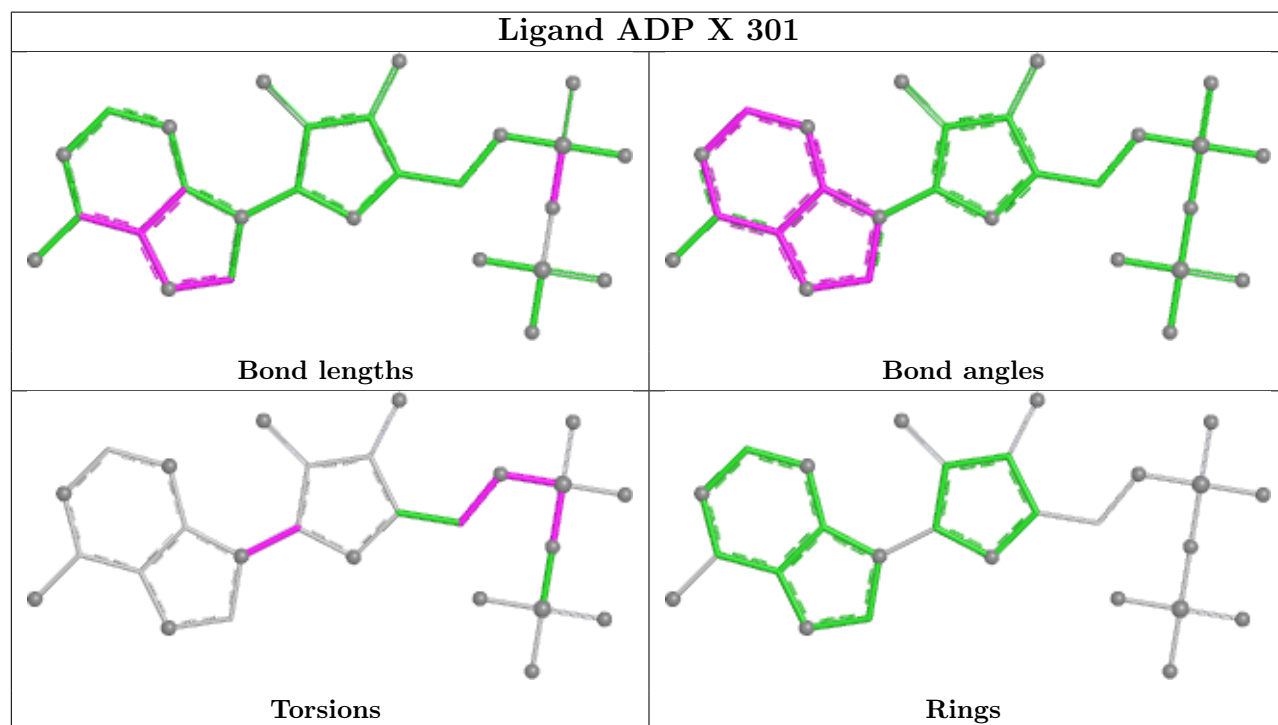
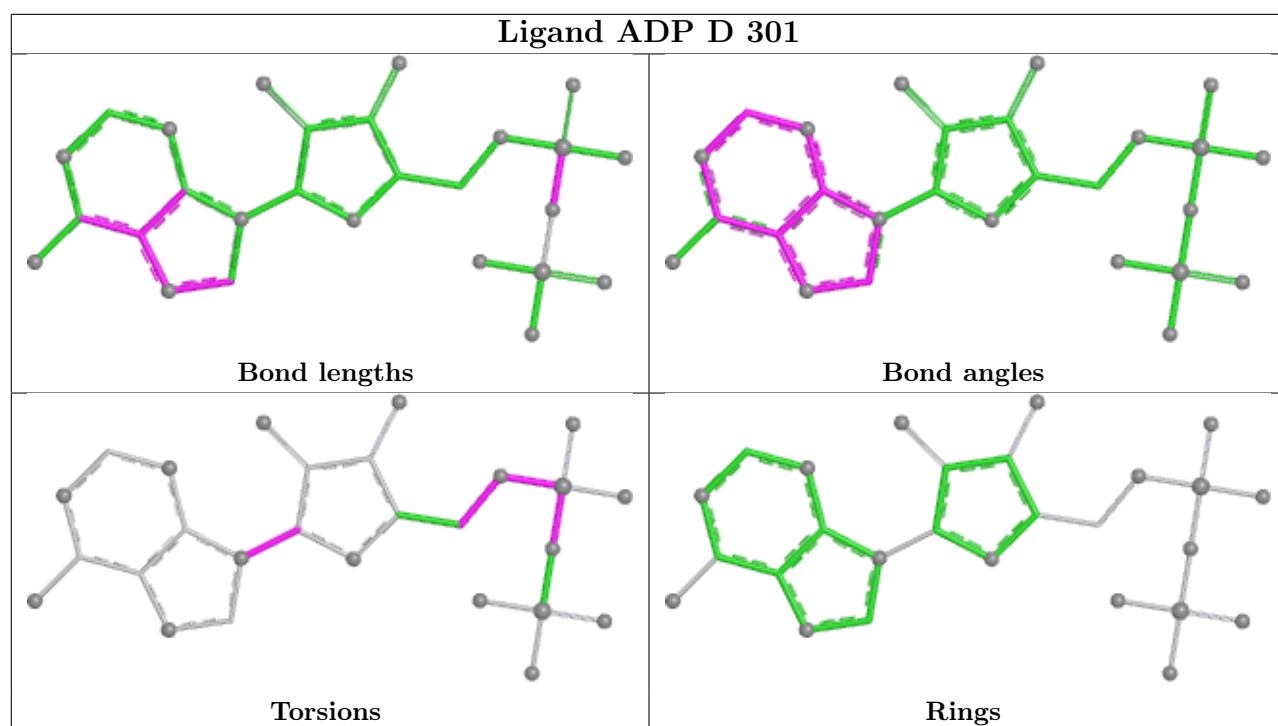


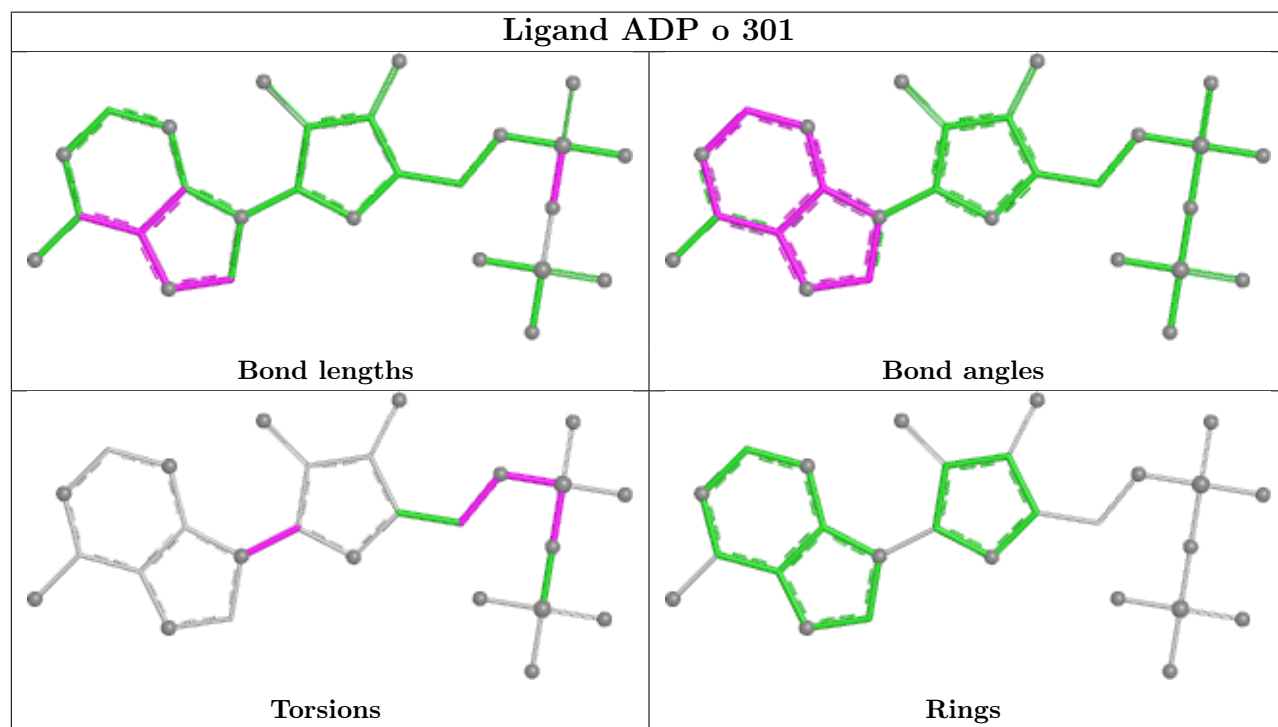
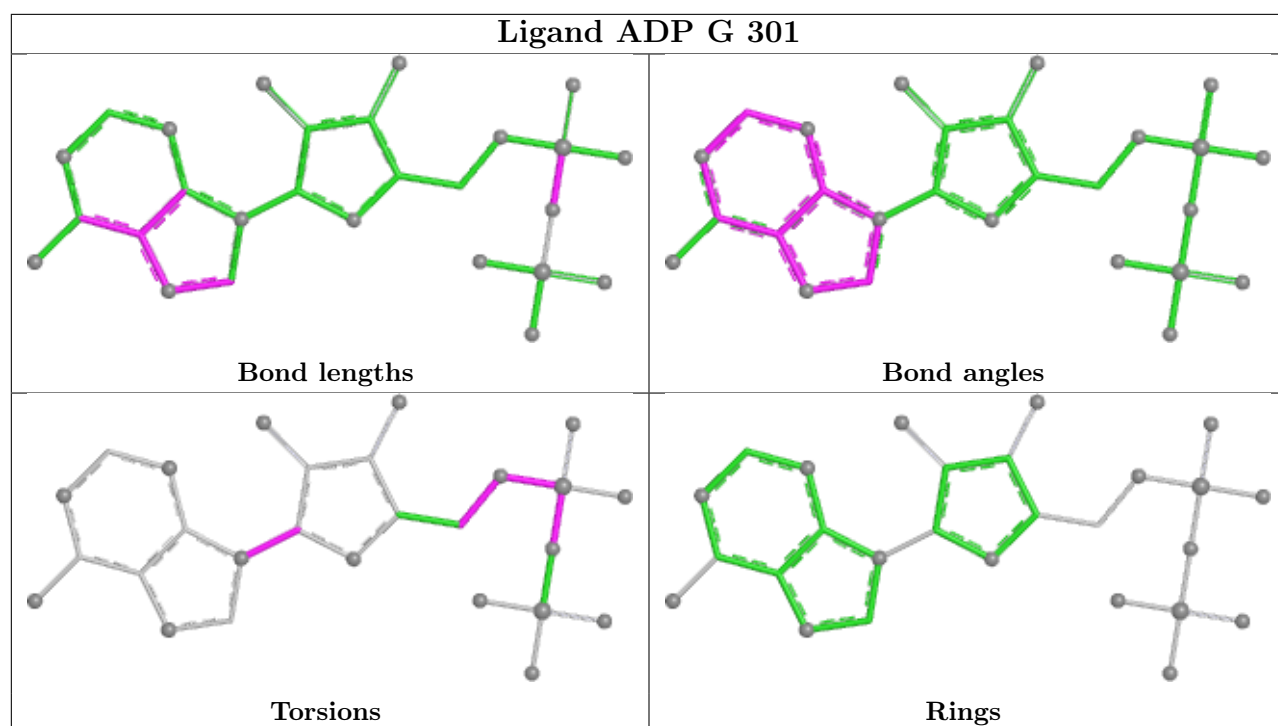


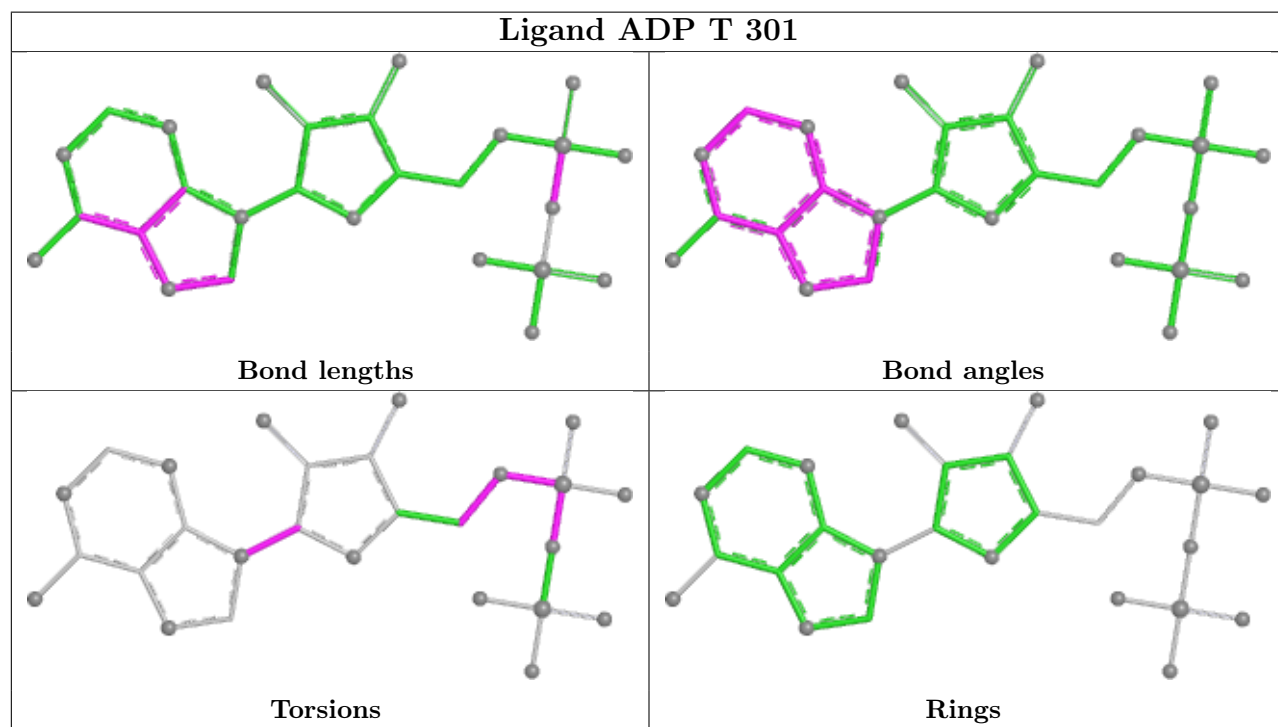
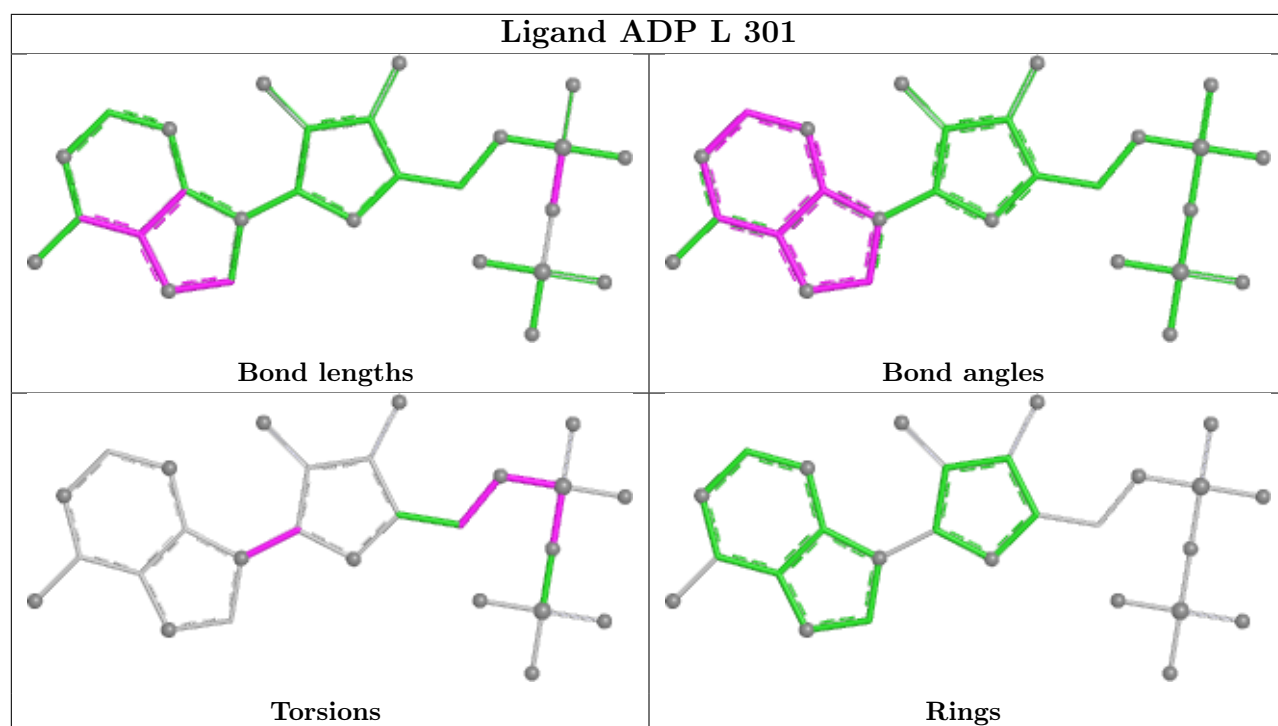




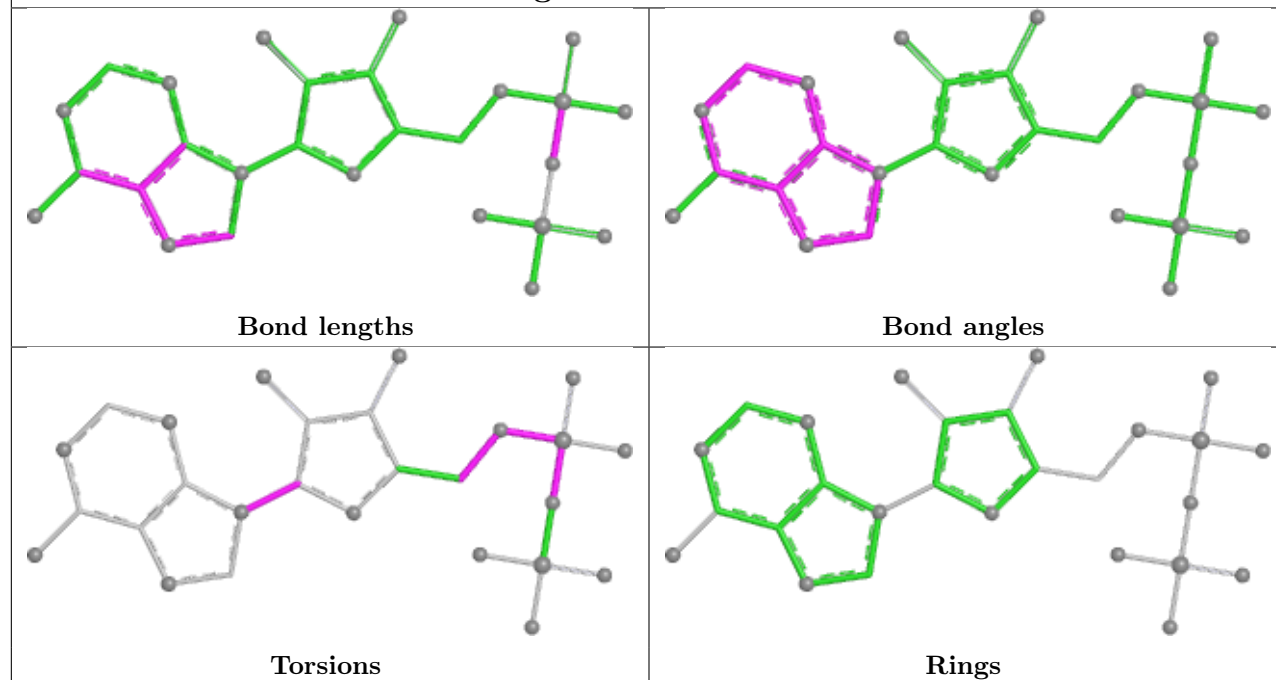




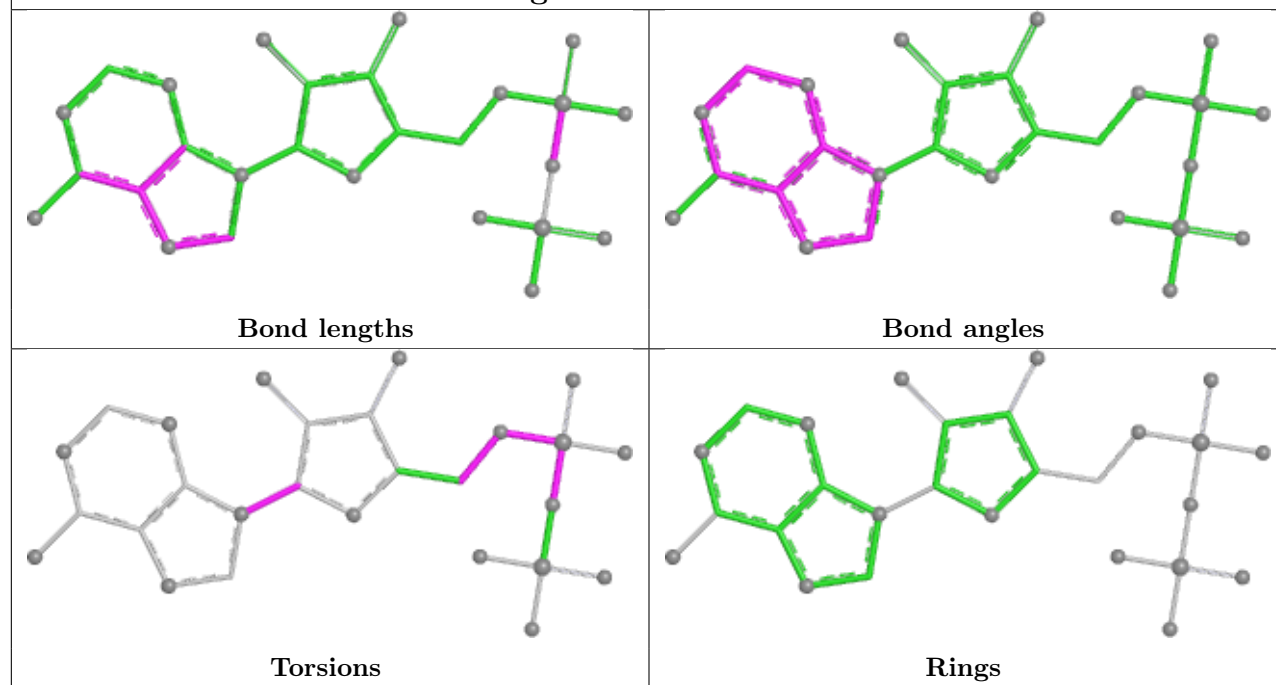


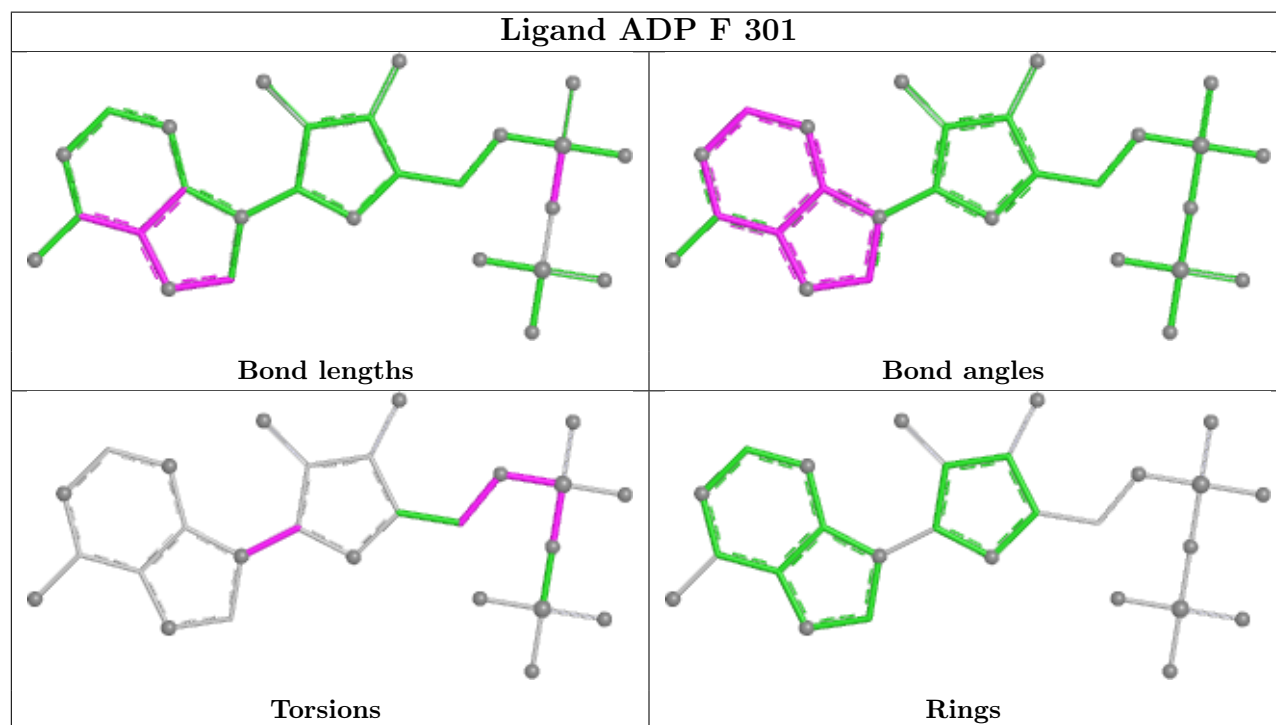
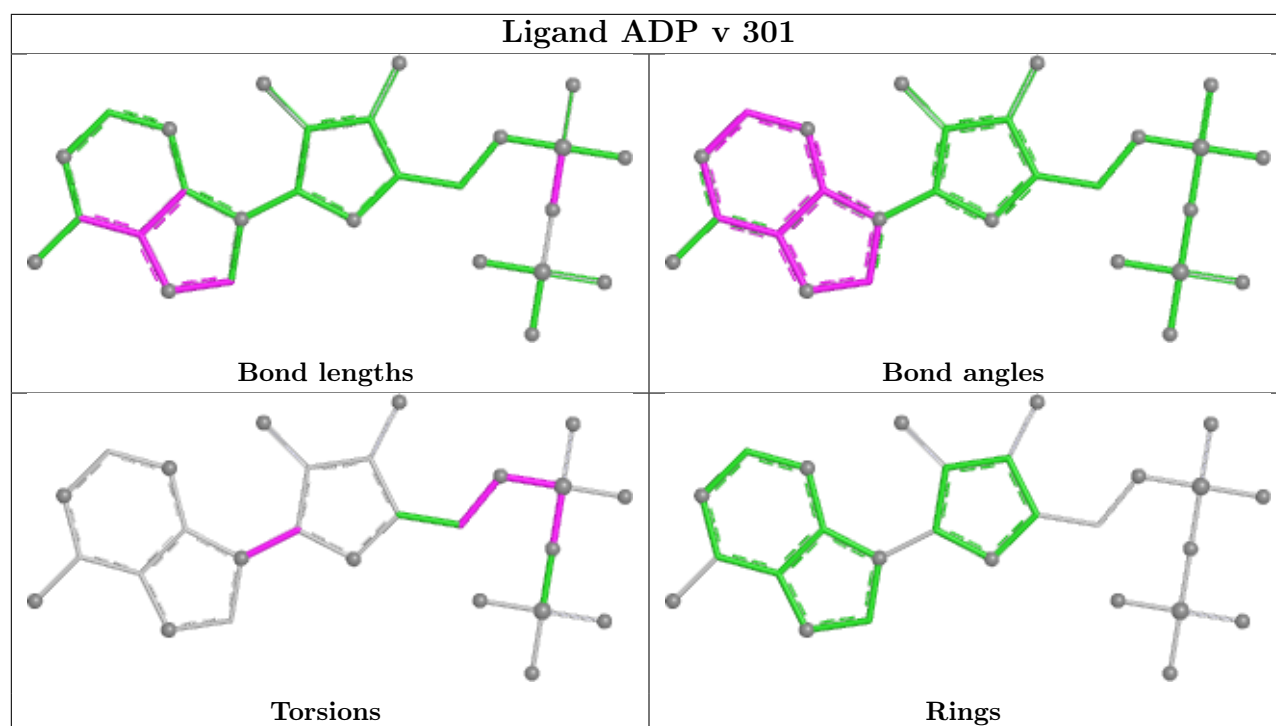


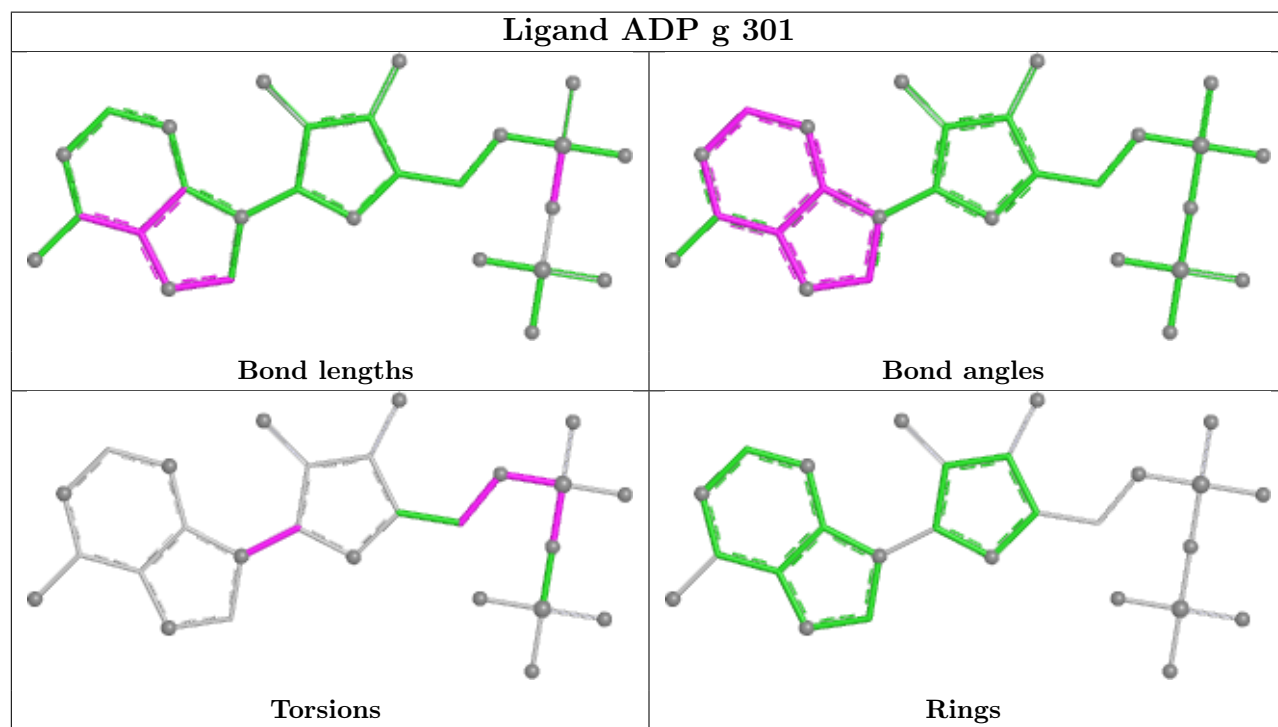
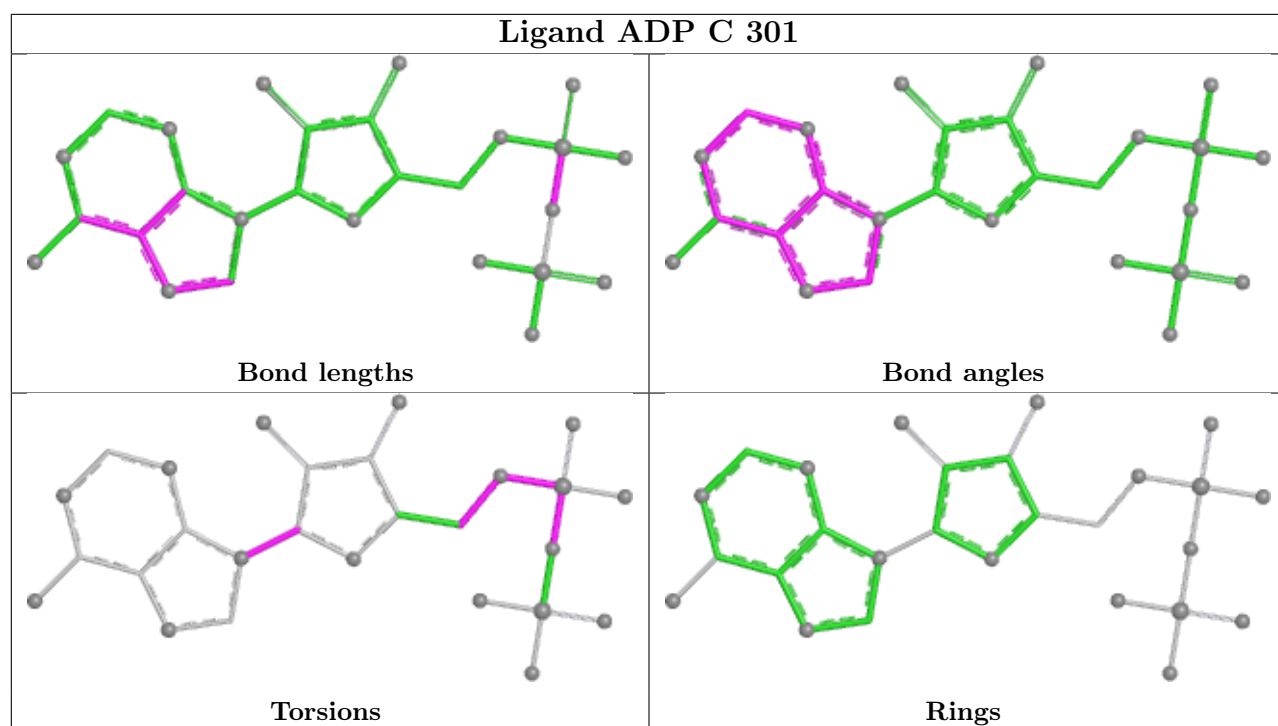
## Ligand ADP 5 301

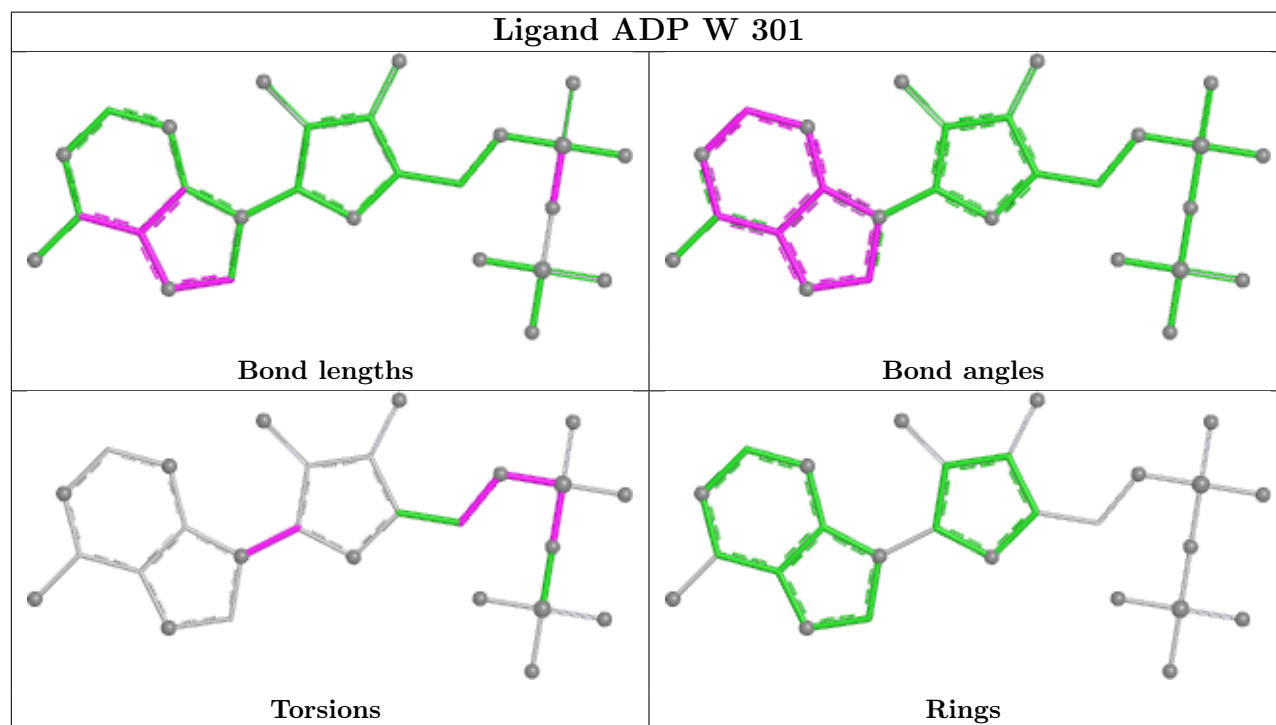
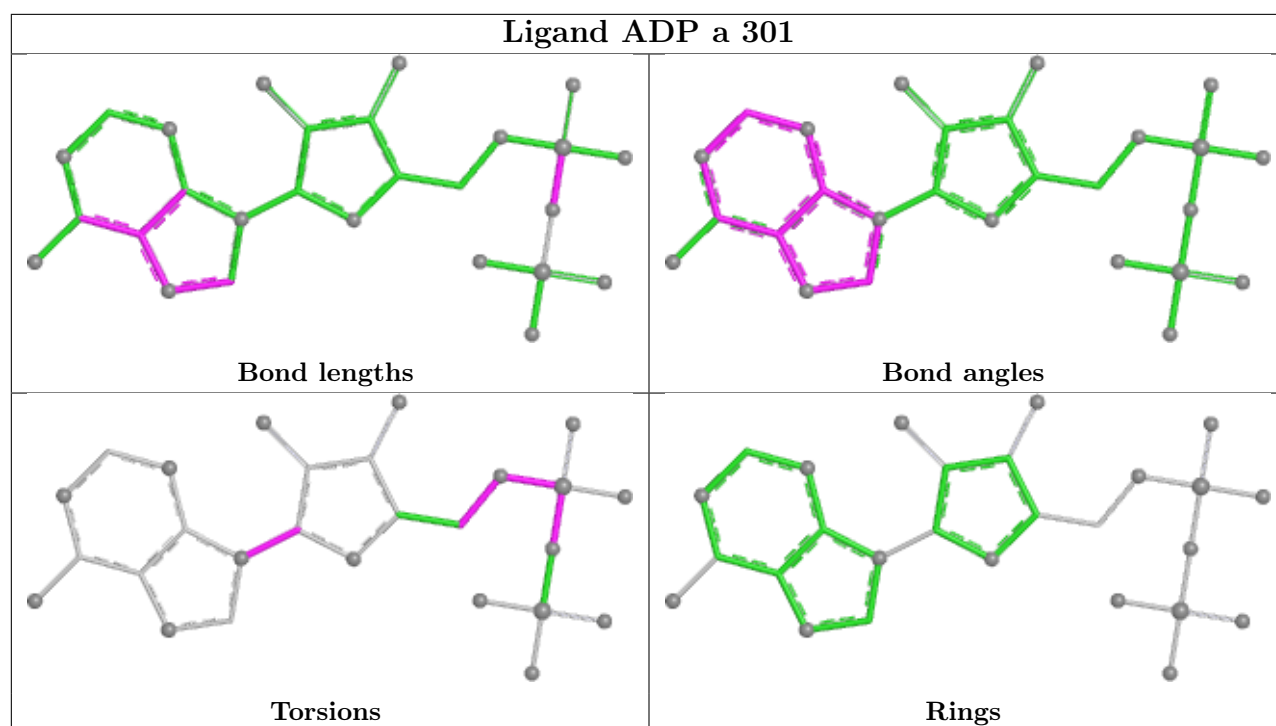


## Ligand ADP B 301

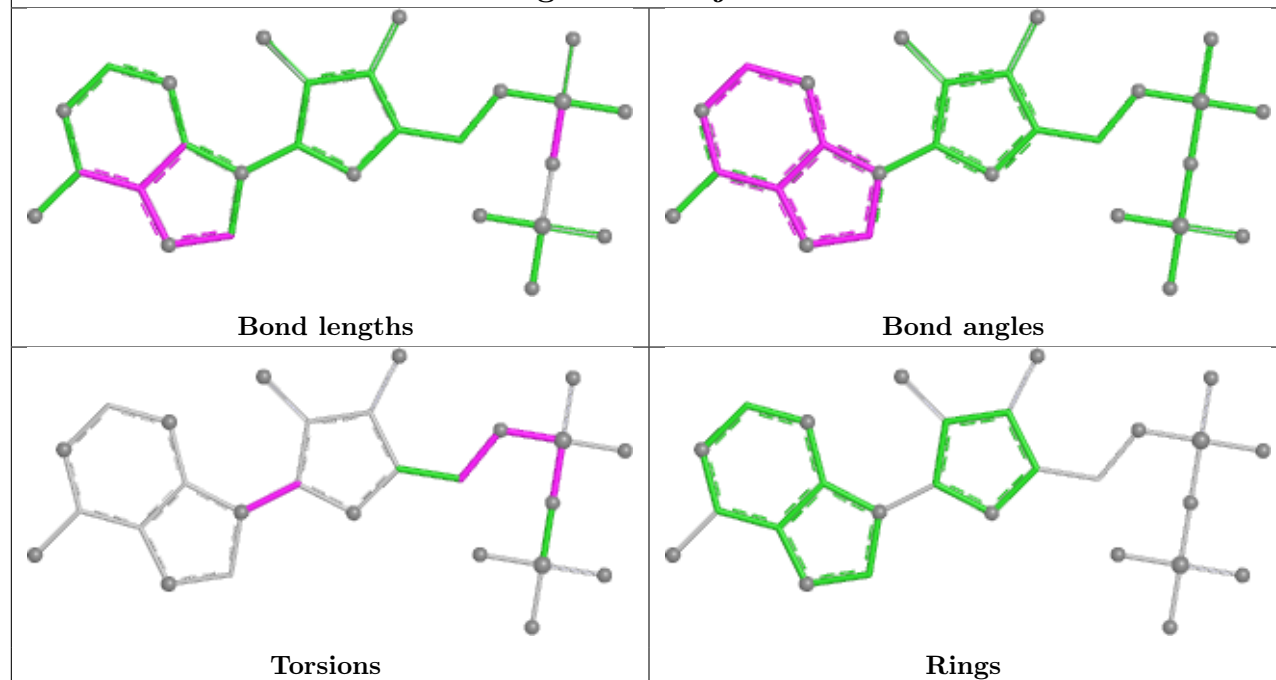




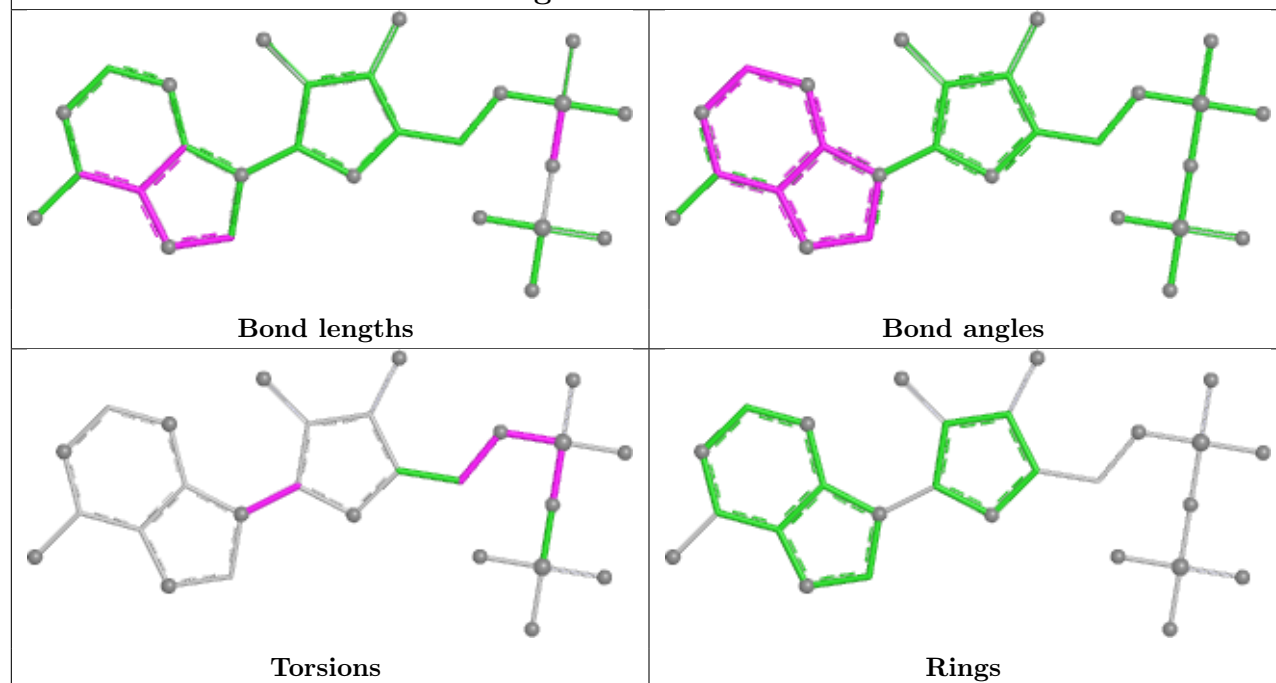


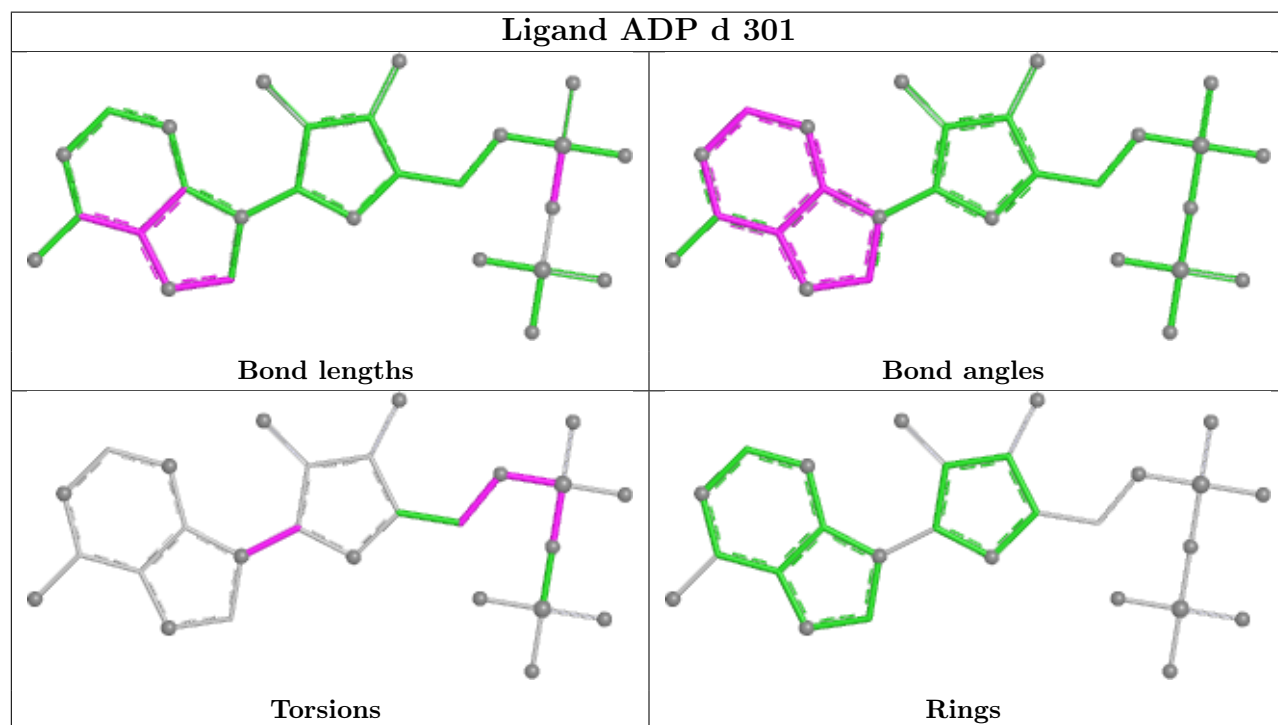
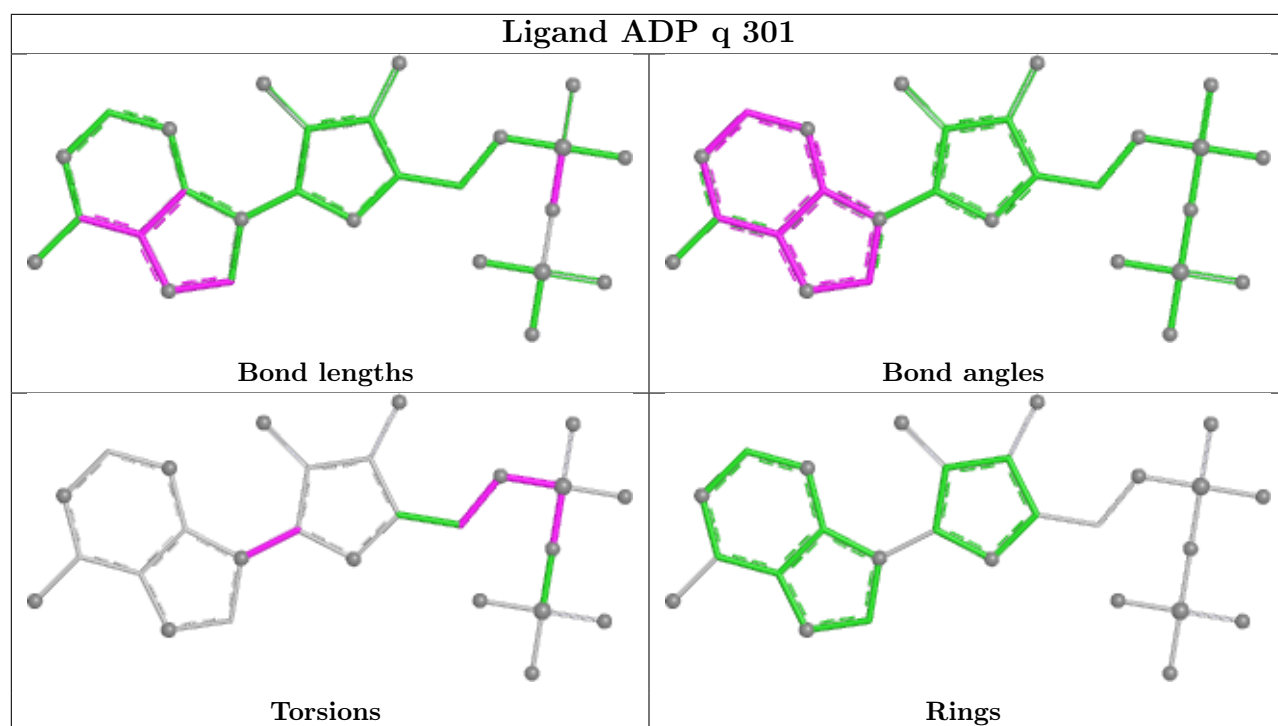


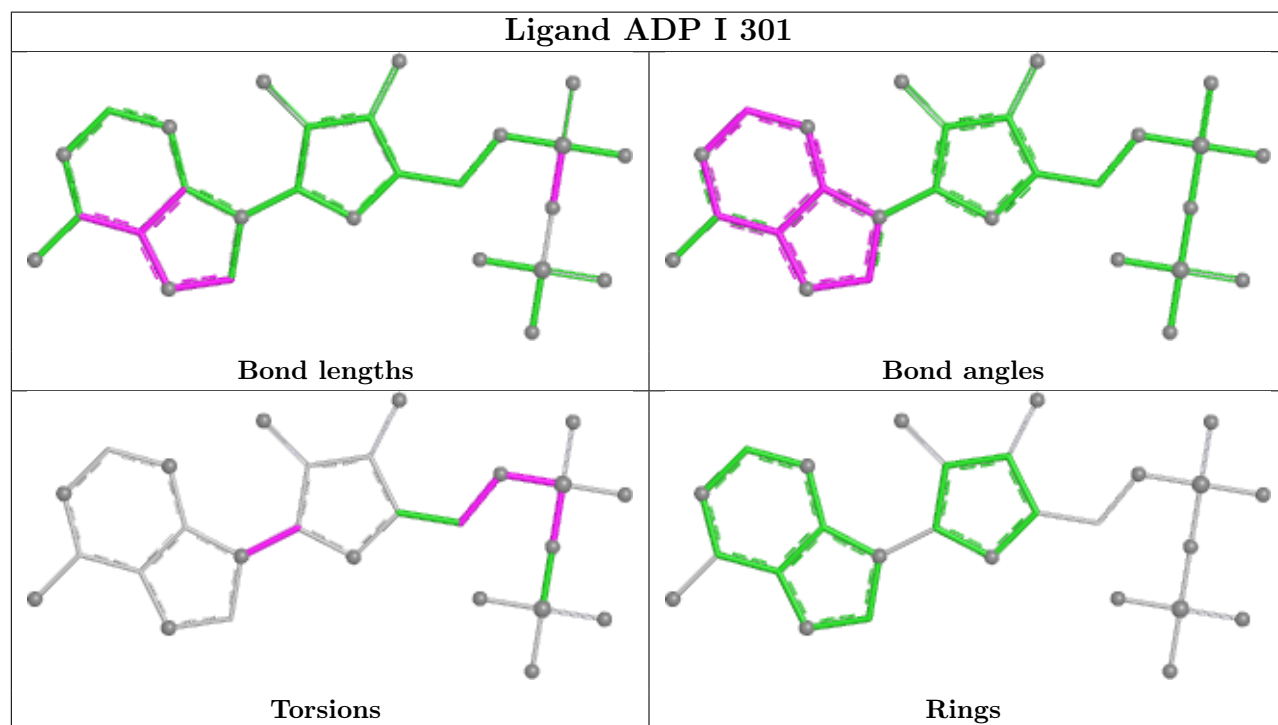
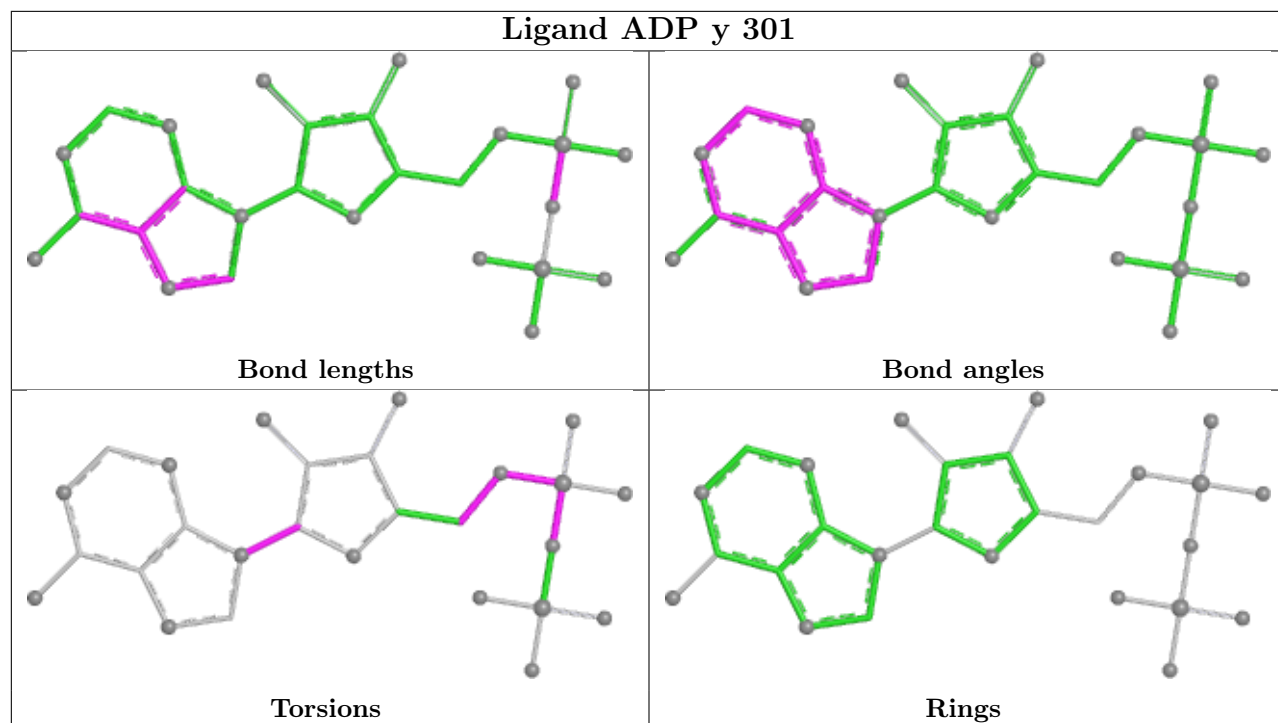
## Ligand ADP j 301

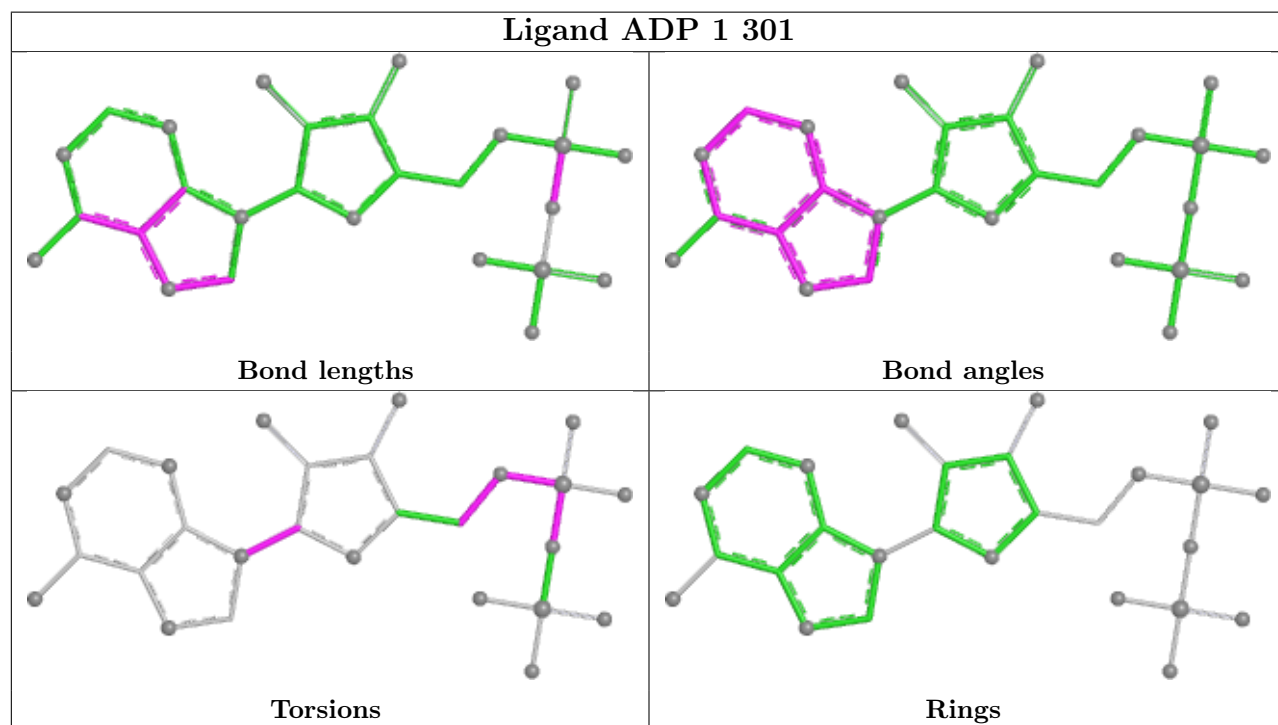
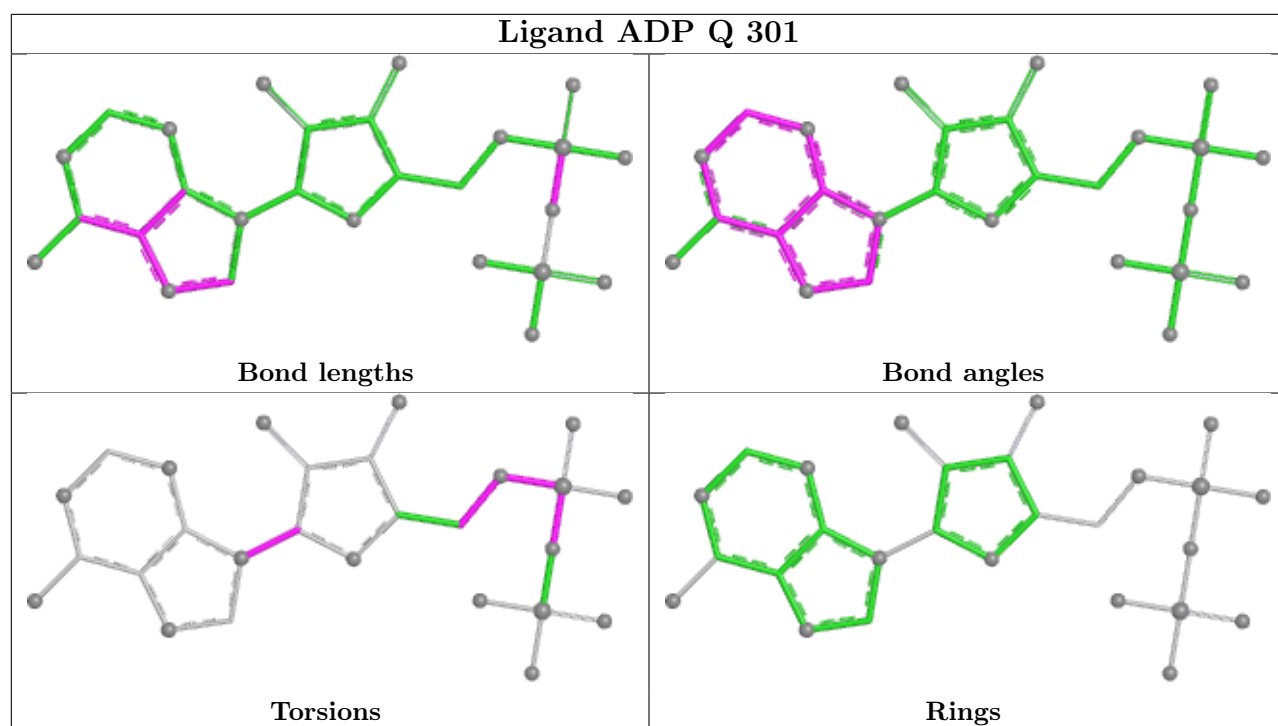


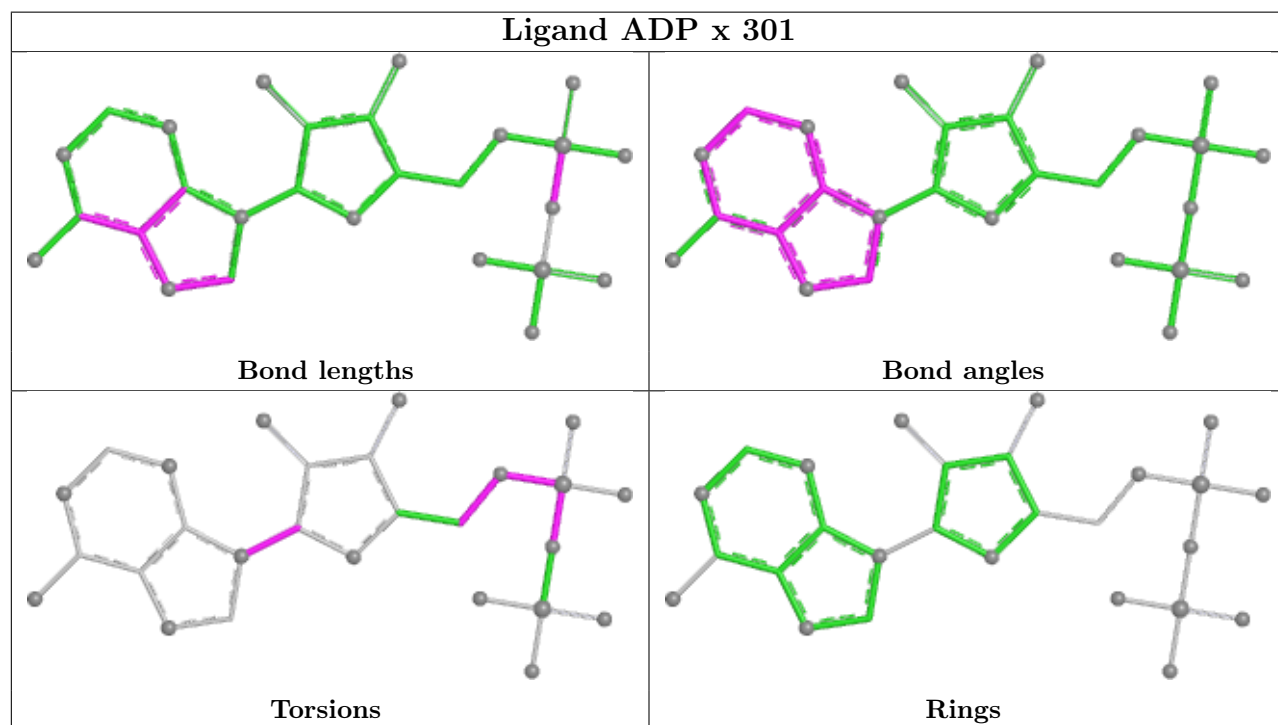
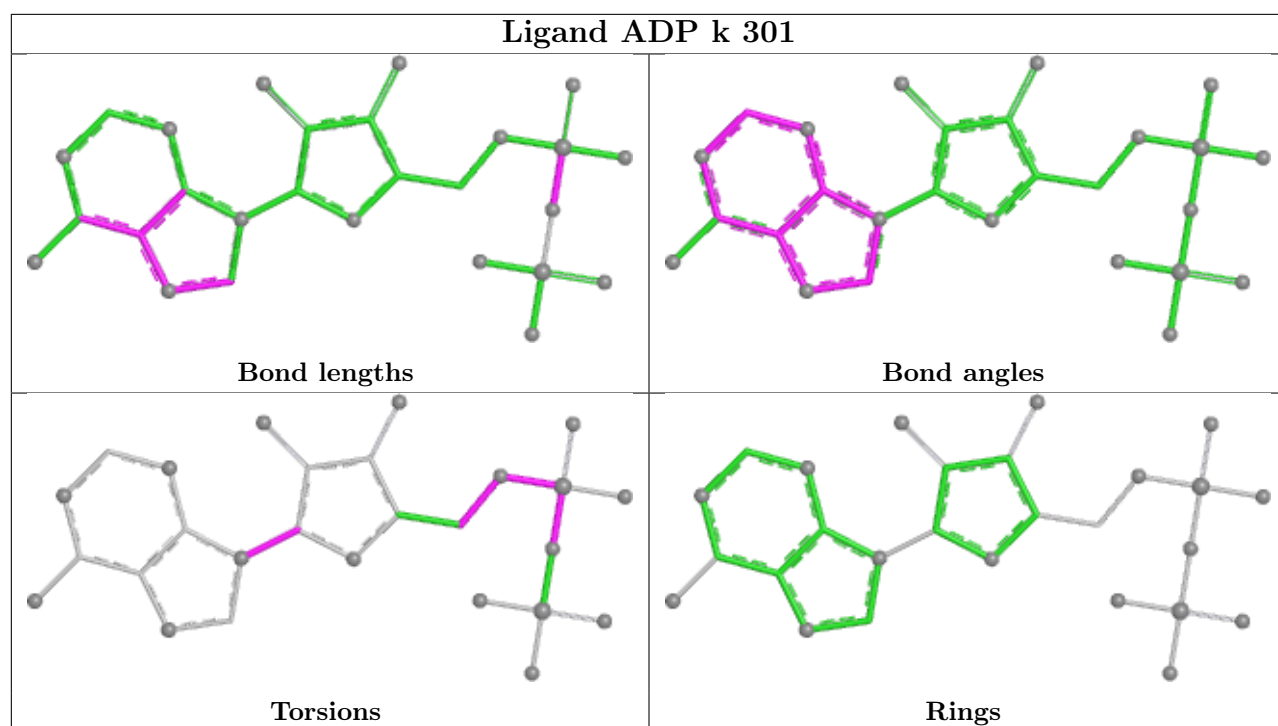
## Ligand ADP 4 301



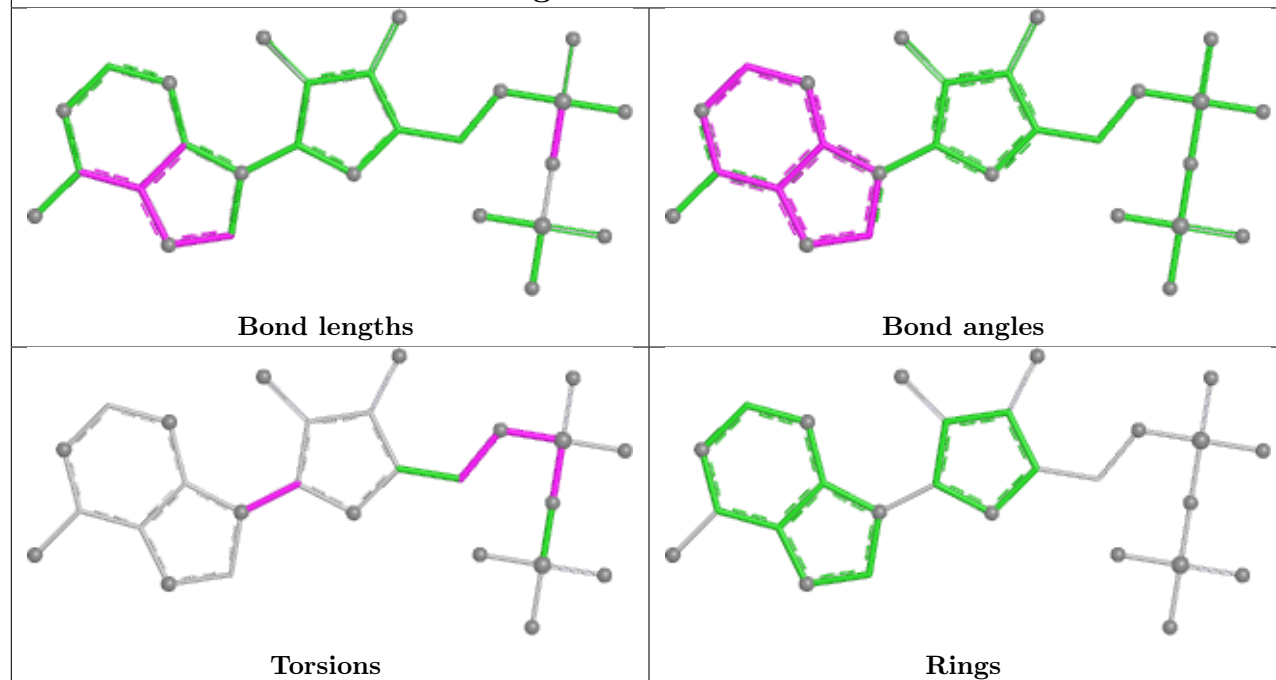




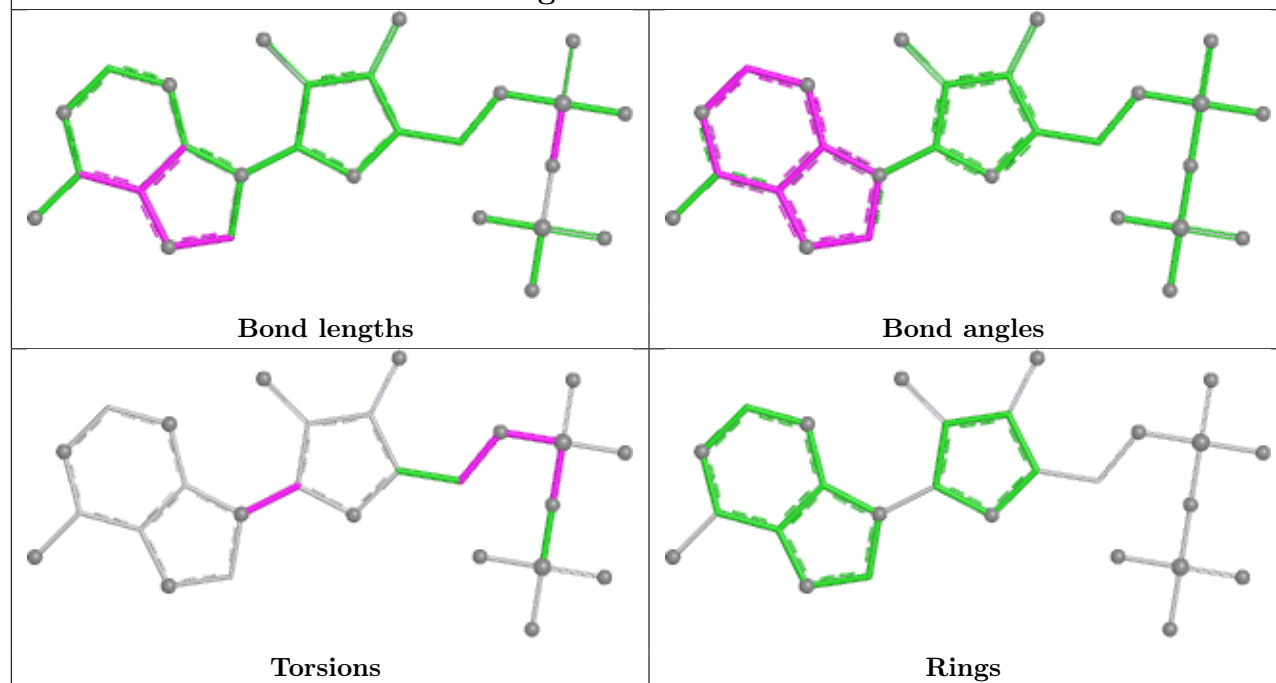




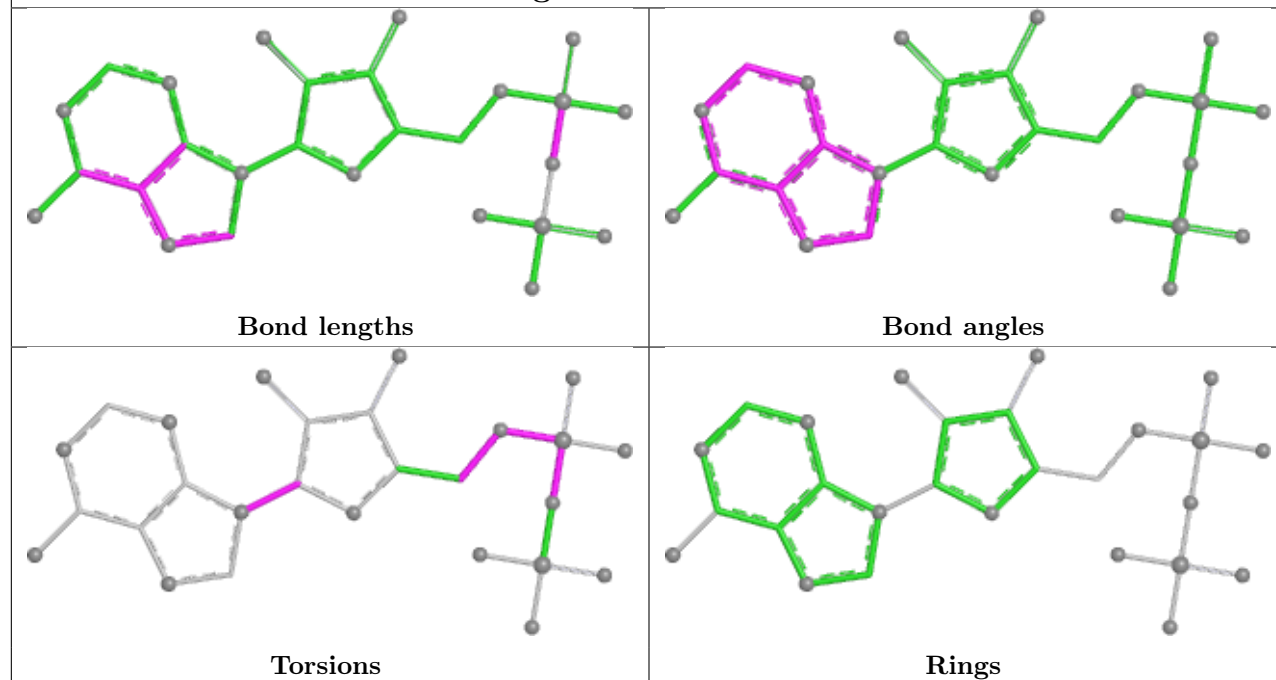
## Ligand ADP b 301



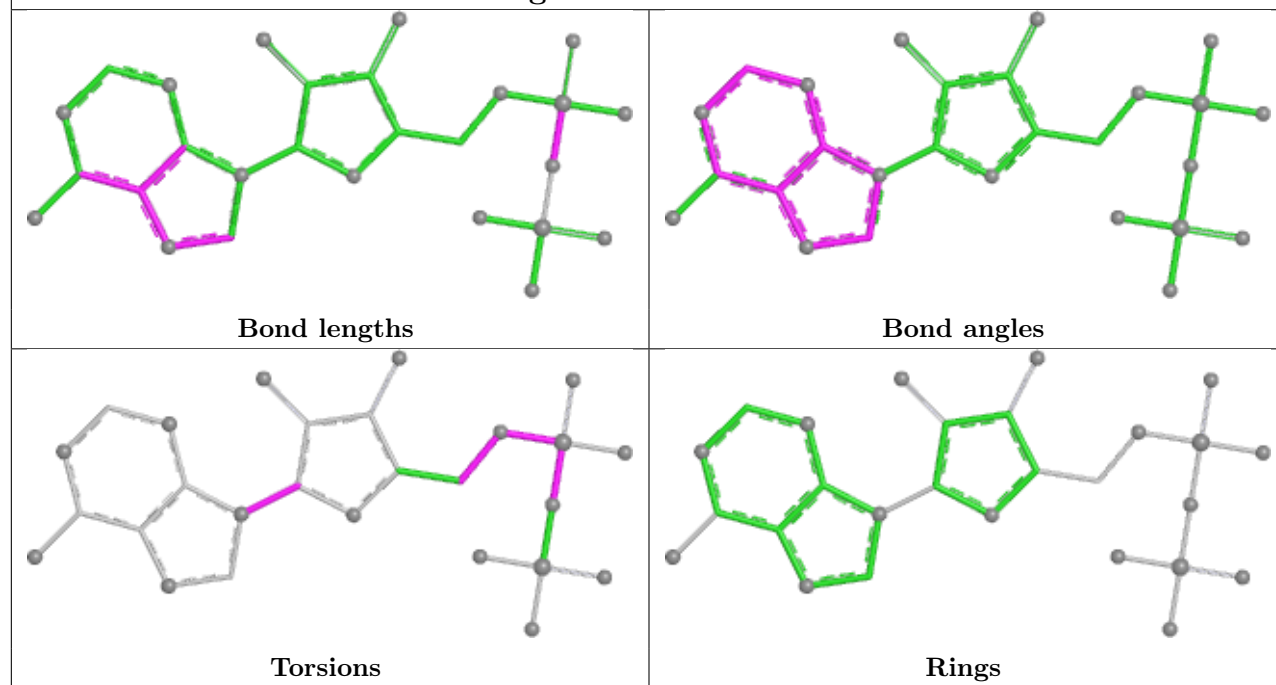
## Ligand ADP l 301

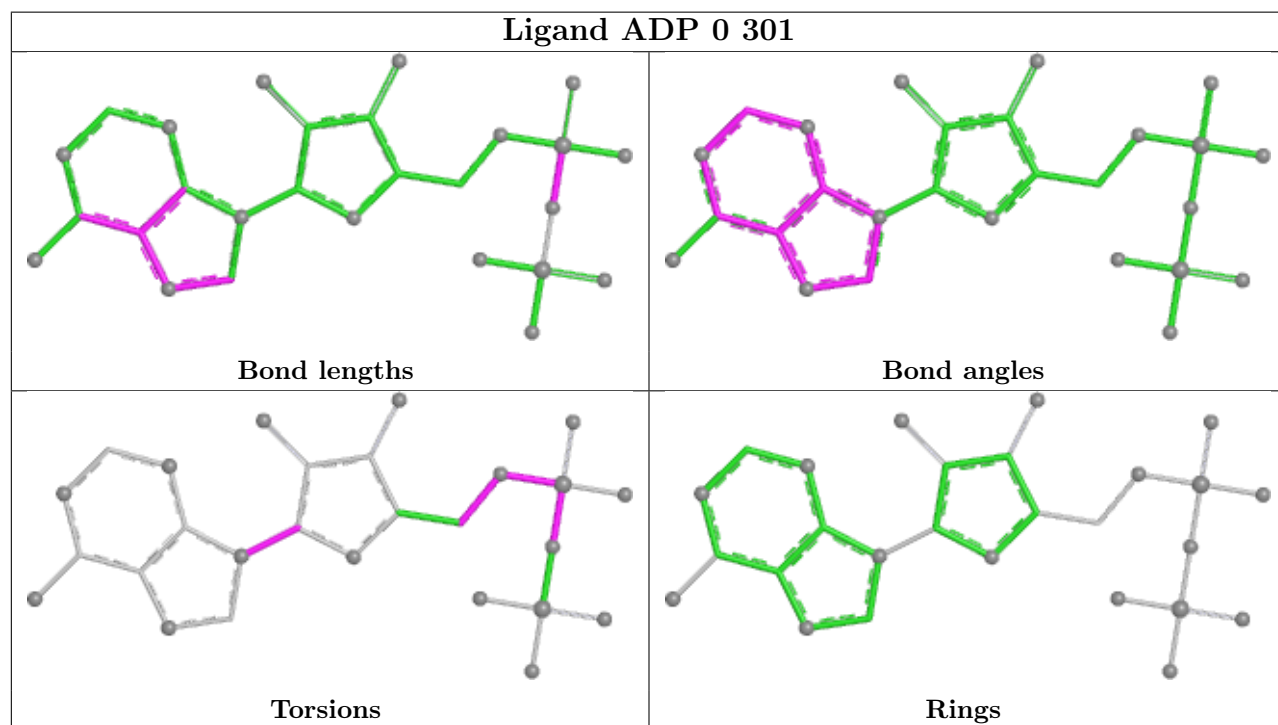
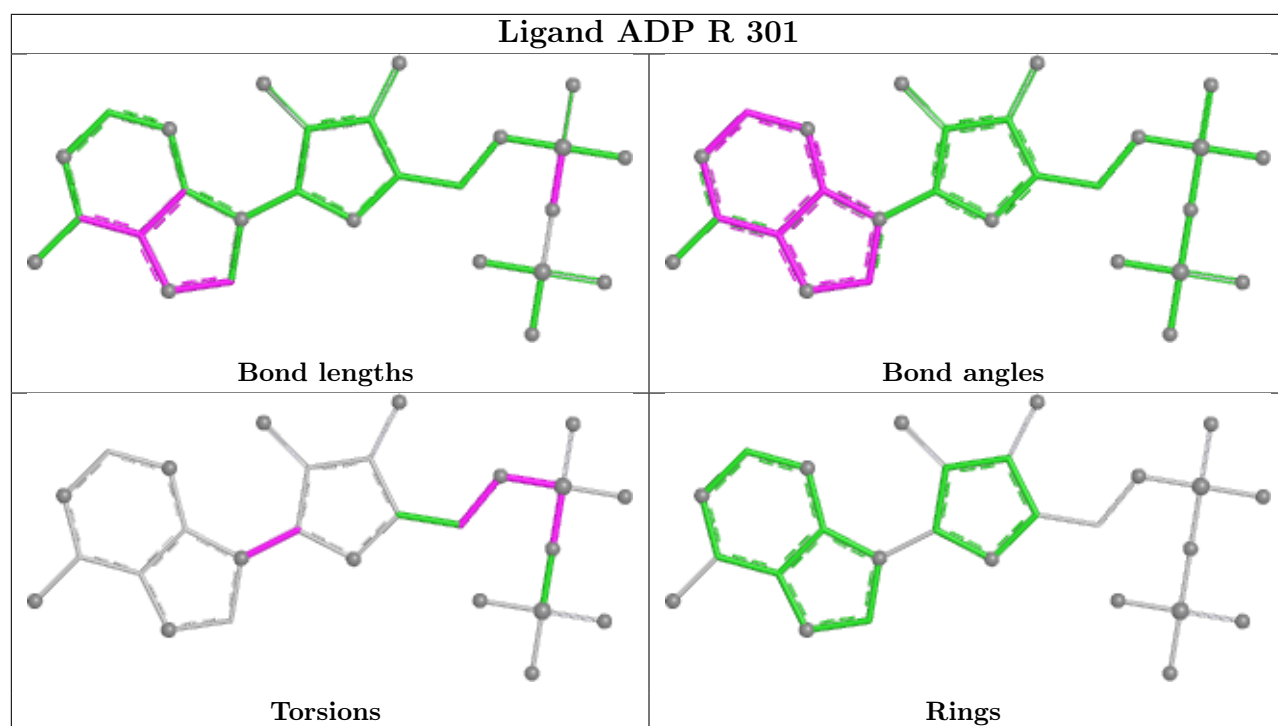


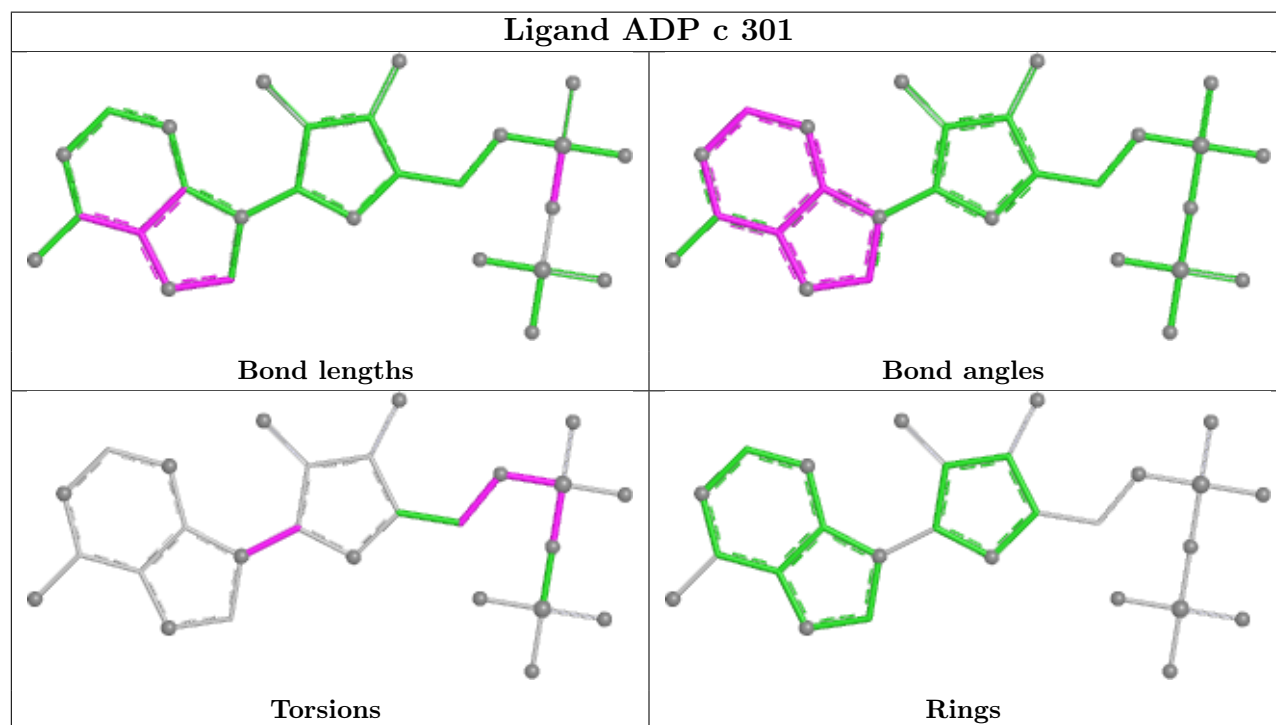
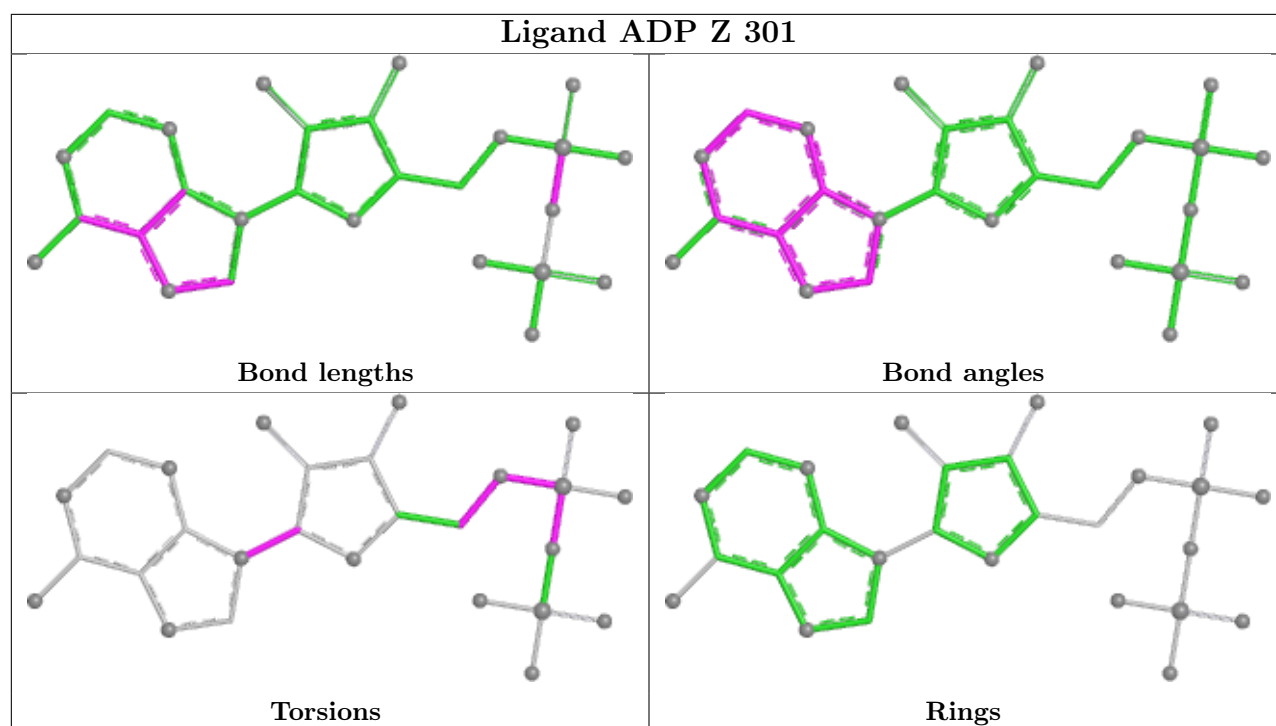
## Ligand ADP h 301



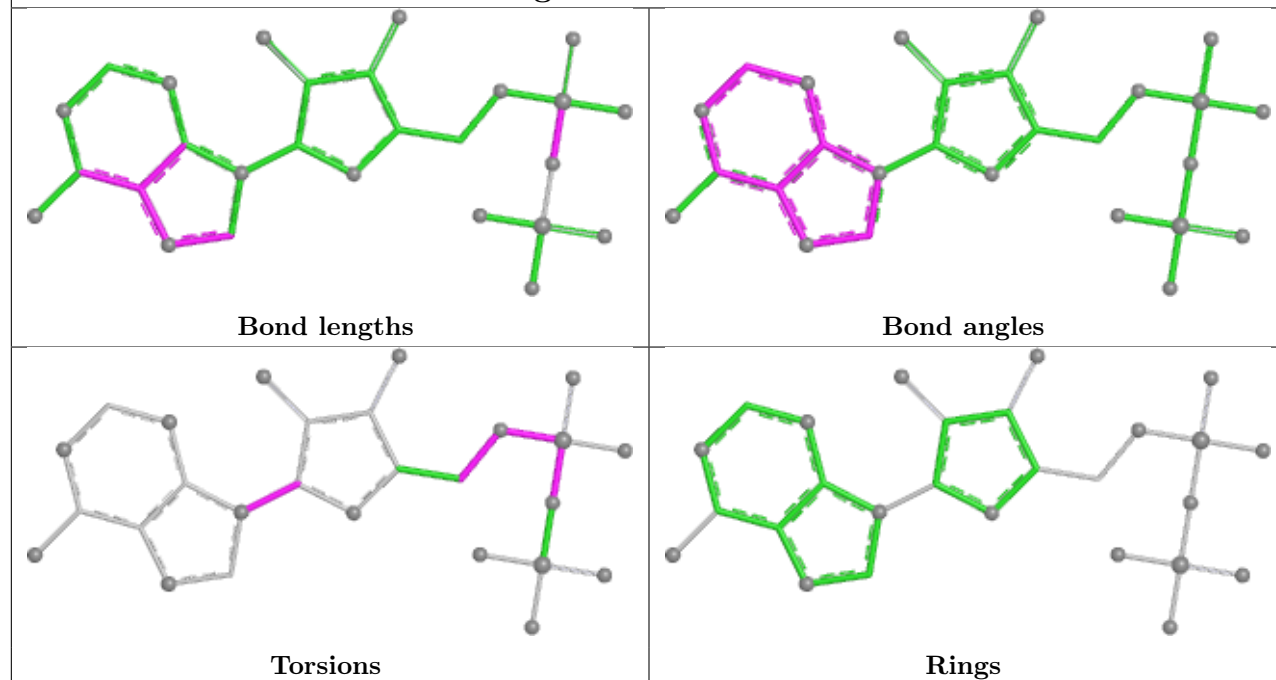
## Ligand ADP K 301



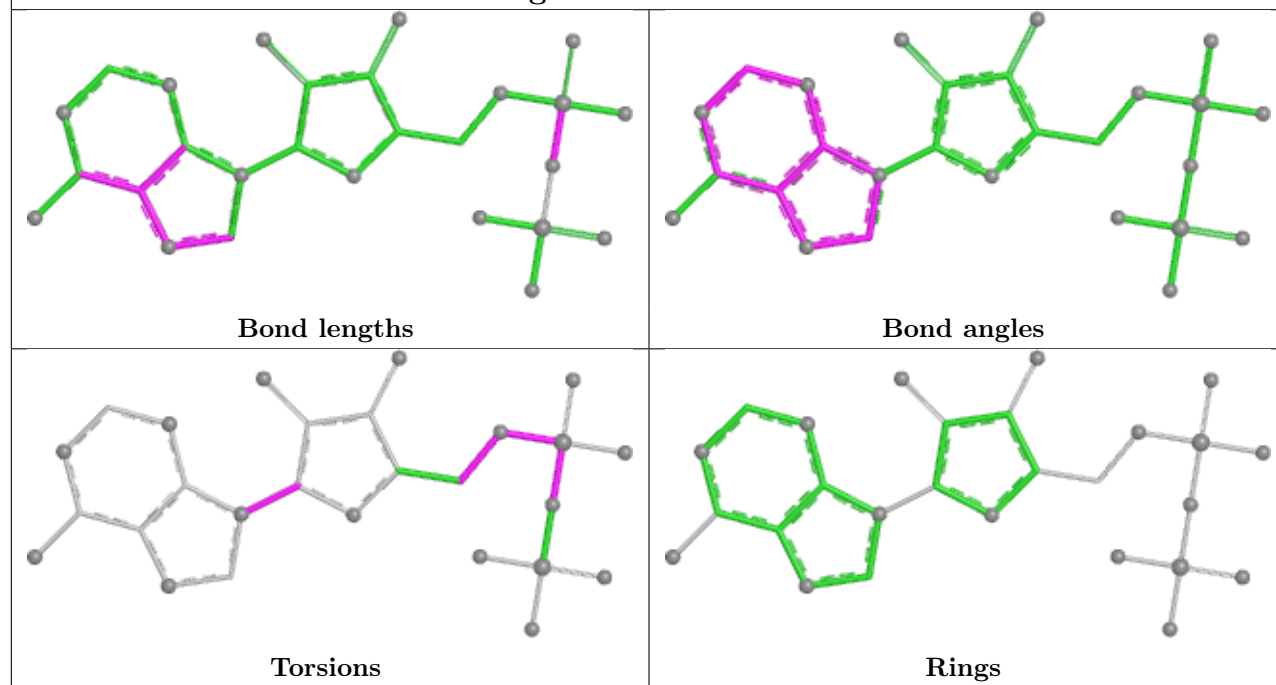


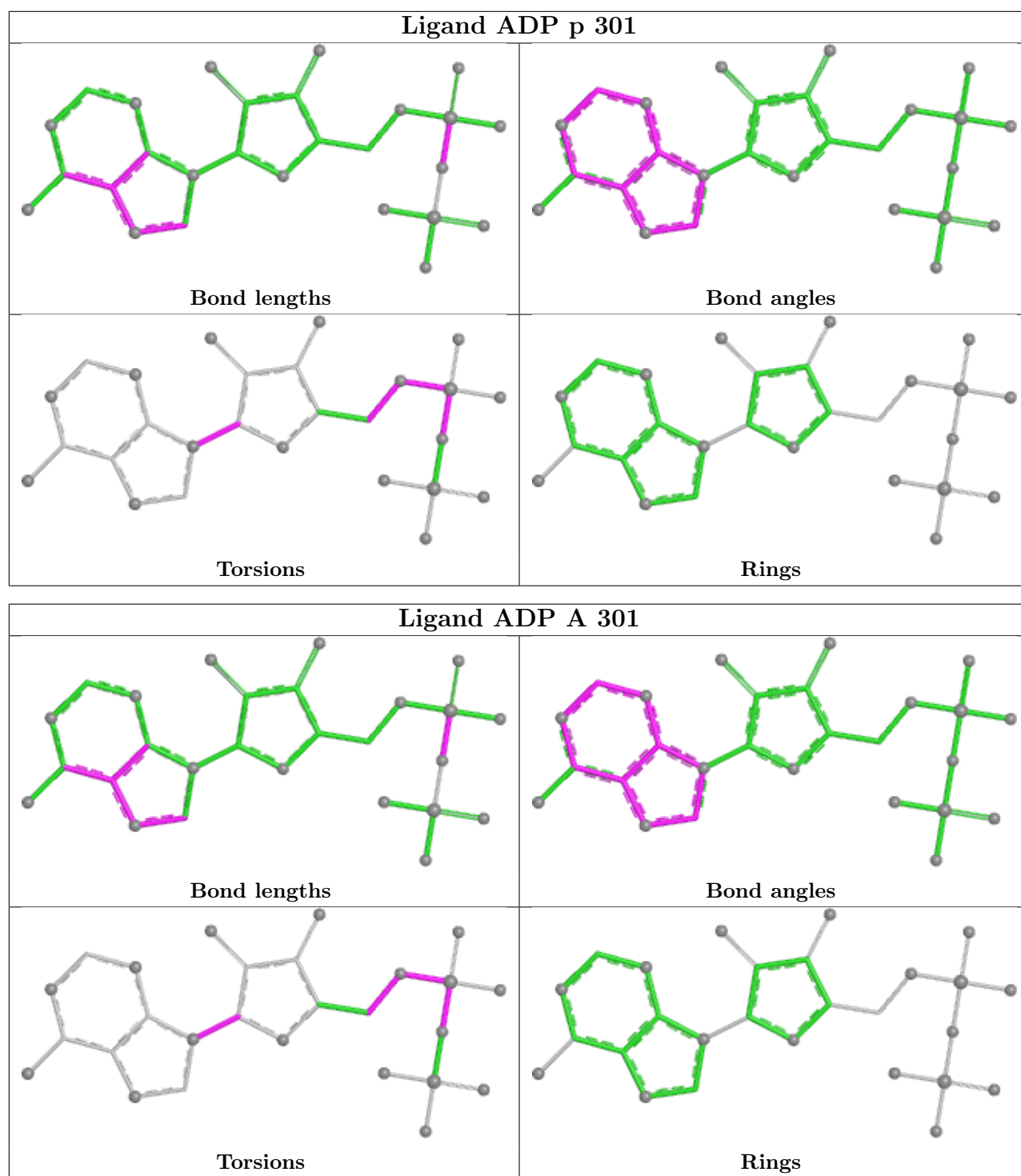


## Ligand ADP 6 301



## Ligand ADP N 301





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

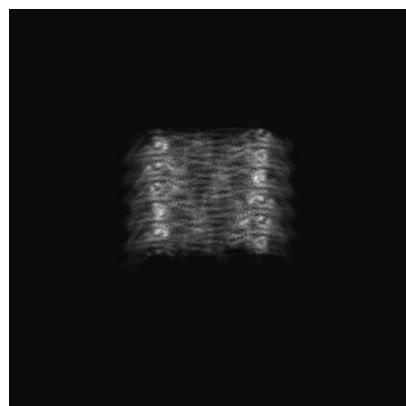
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15491. These allow visual inspection of the internal detail of the map and identification of artifacts.

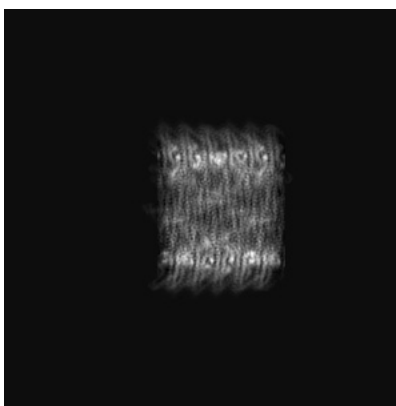
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

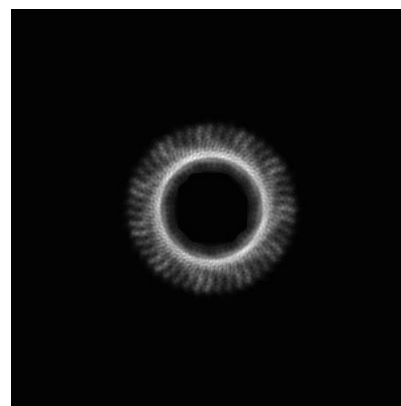
#### 6.1.1 Primary map



X

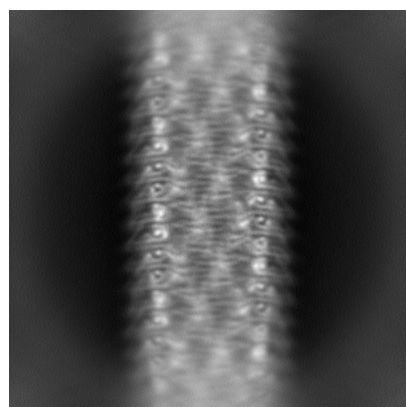


Y

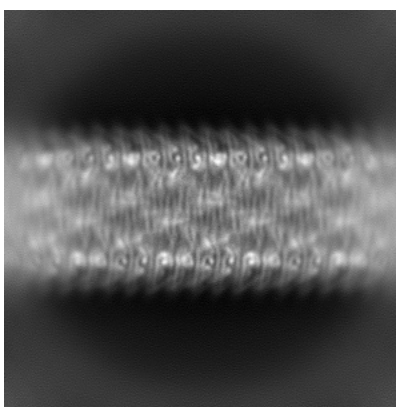


Z

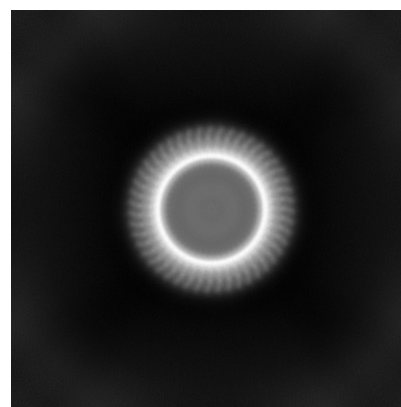
#### 6.1.2 Raw map



X



Y

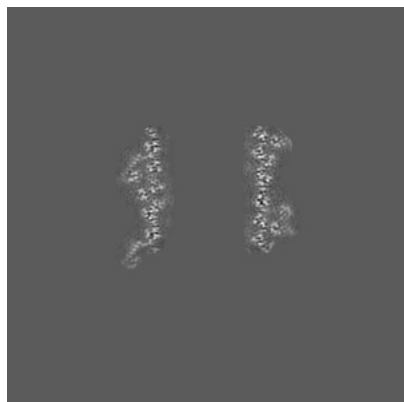


Z

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

## 6.2 Central slices [i](#)

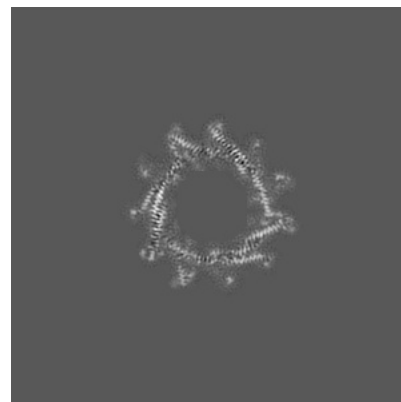
### 6.2.1 Primary map



X Index: 200

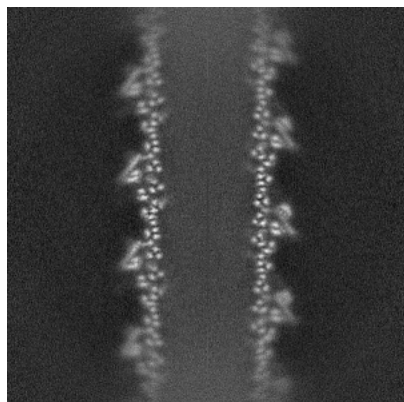


Y Index: 200

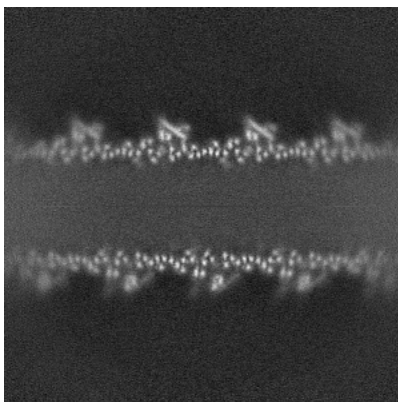


Z Index: 200

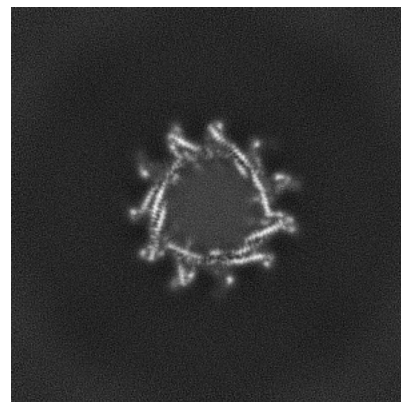
### 6.2.2 Raw map



X Index: 200



Y Index: 200

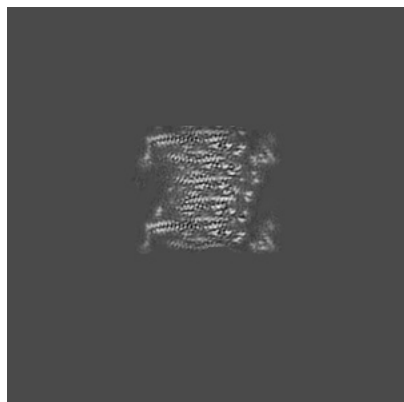


Z Index: 200

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

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

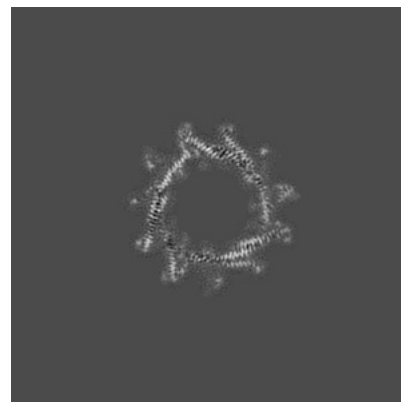
### 6.3.1 Primary map



X Index: 148

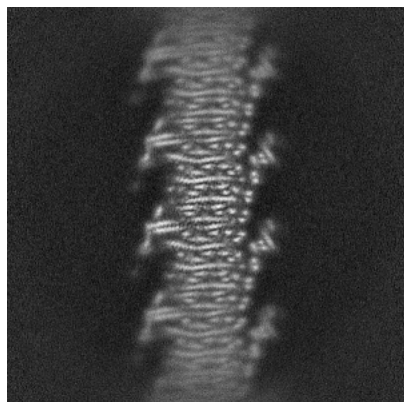


Y Index: 252

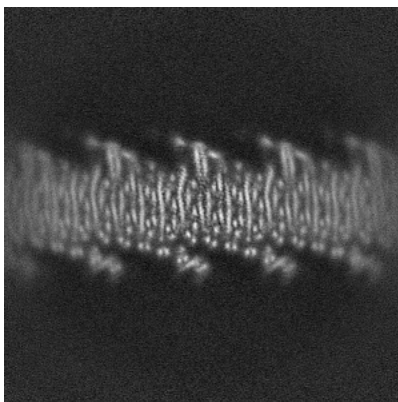


Z Index: 222

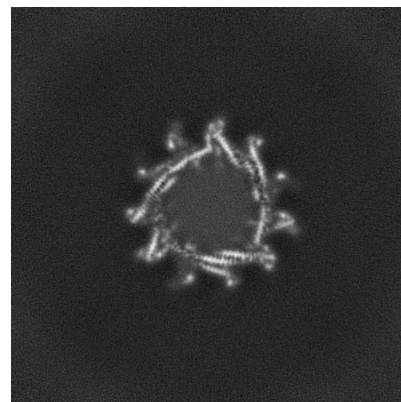
### 6.3.2 Raw map



X Index: 148



Y Index: 148

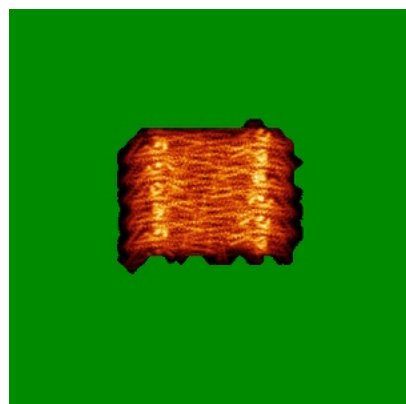


Z Index: 196

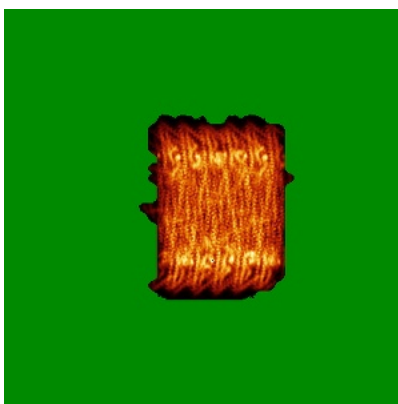
The images above show the largest variance slices of the map in three orthogonal directions.

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

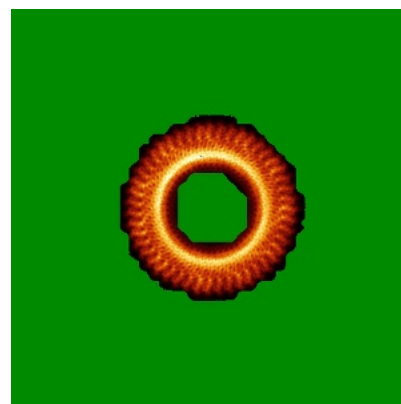
### 6.4.1 Primary map



X

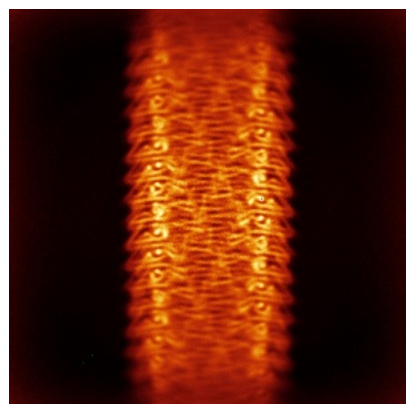


Y

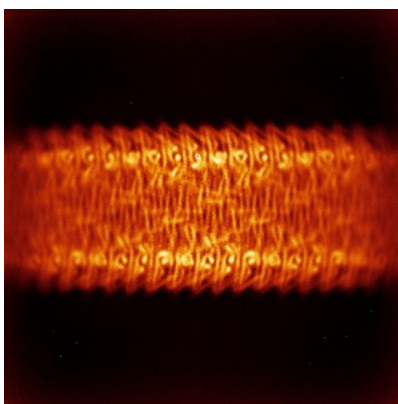


Z

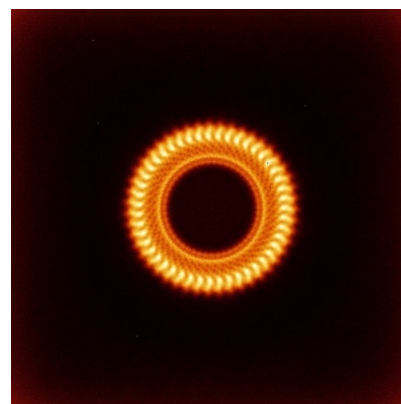
### 6.4.2 Raw map



X



Y

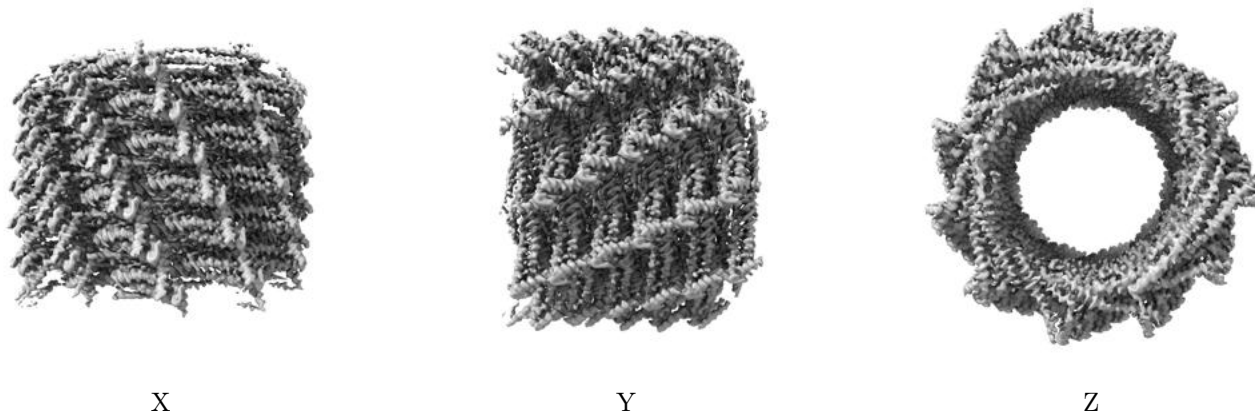


Z

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.

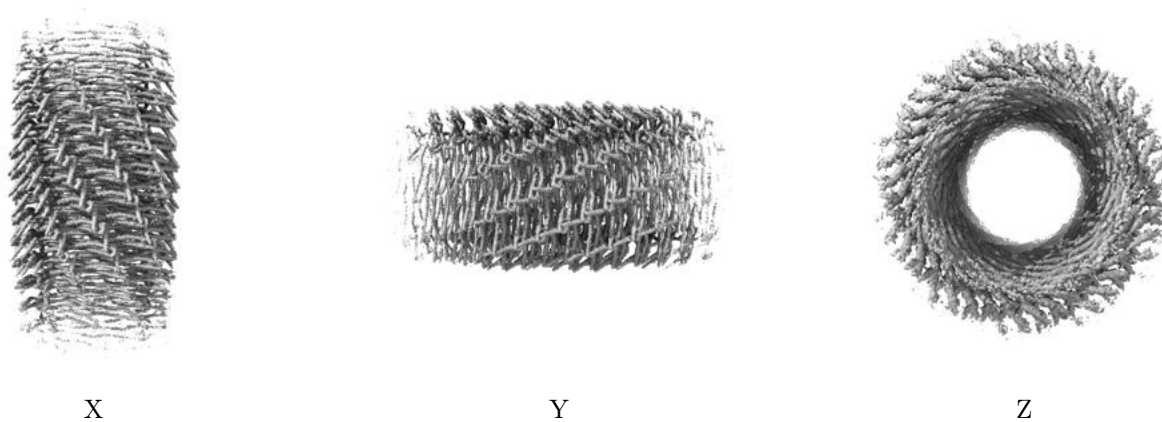
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

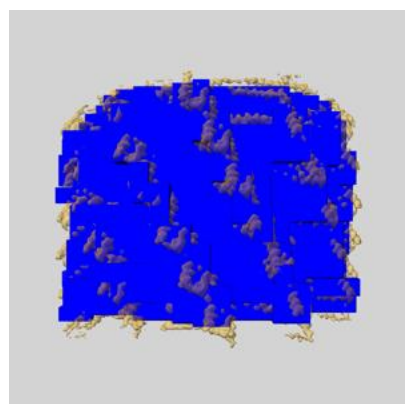
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

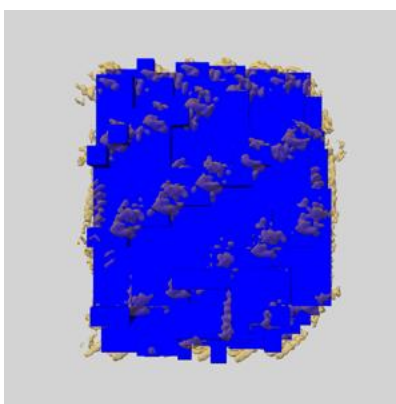
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

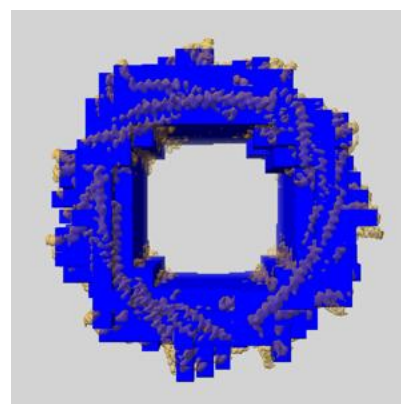
### 6.6.1 emd\_15491\_msk\_1.map [i](#)



X



Y

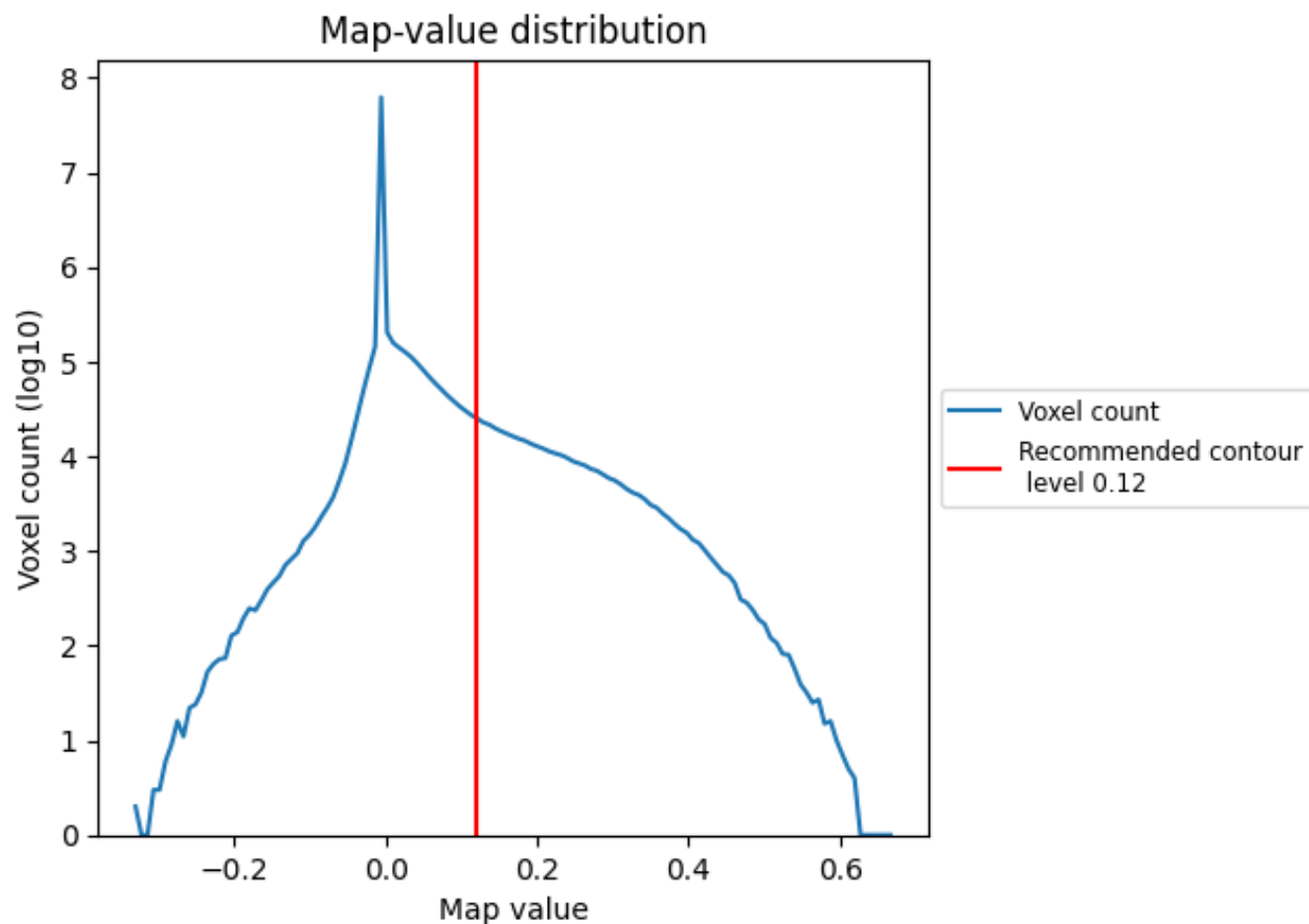


Z

## 7 Map analysis [i](#)

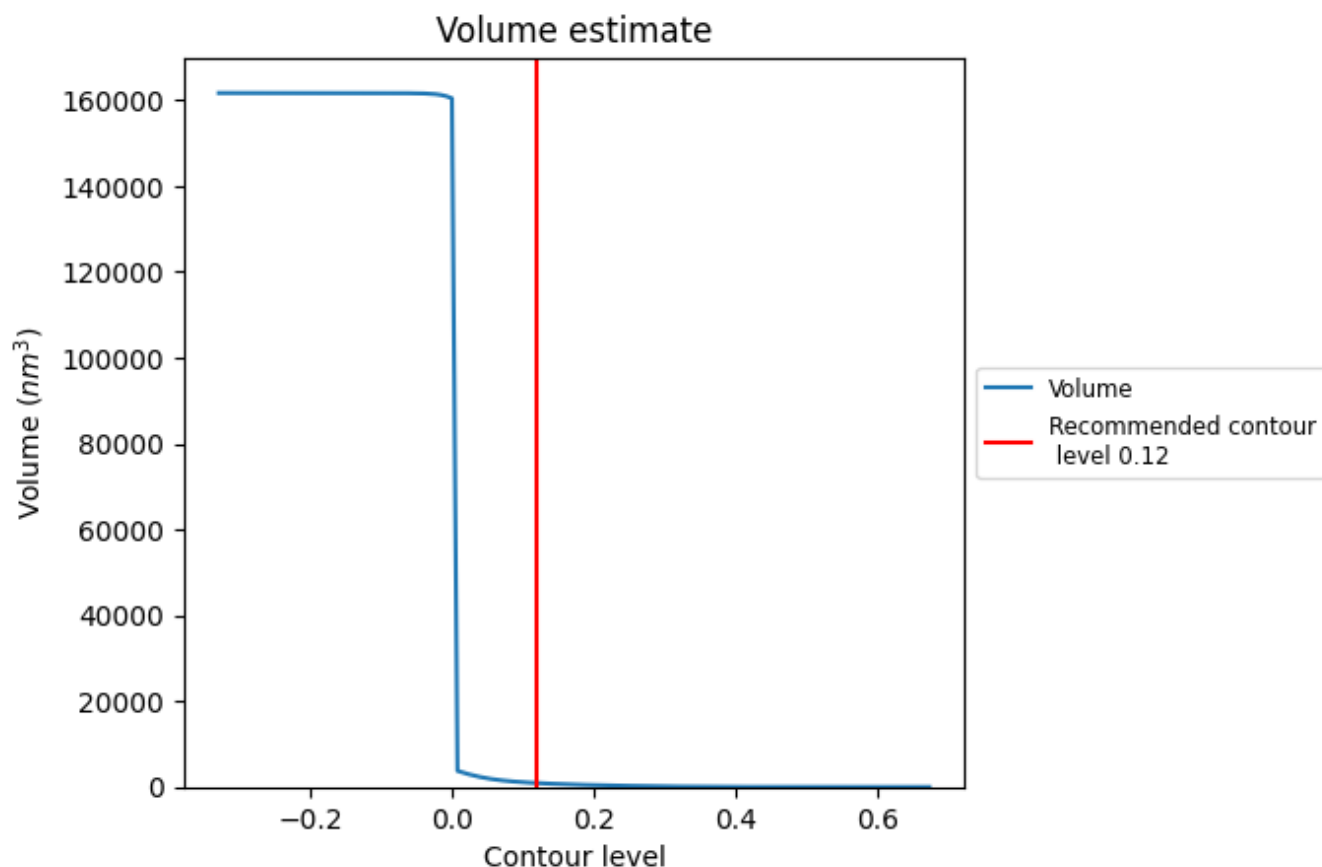
This section contains the results of statistical analysis of the map.

### 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.

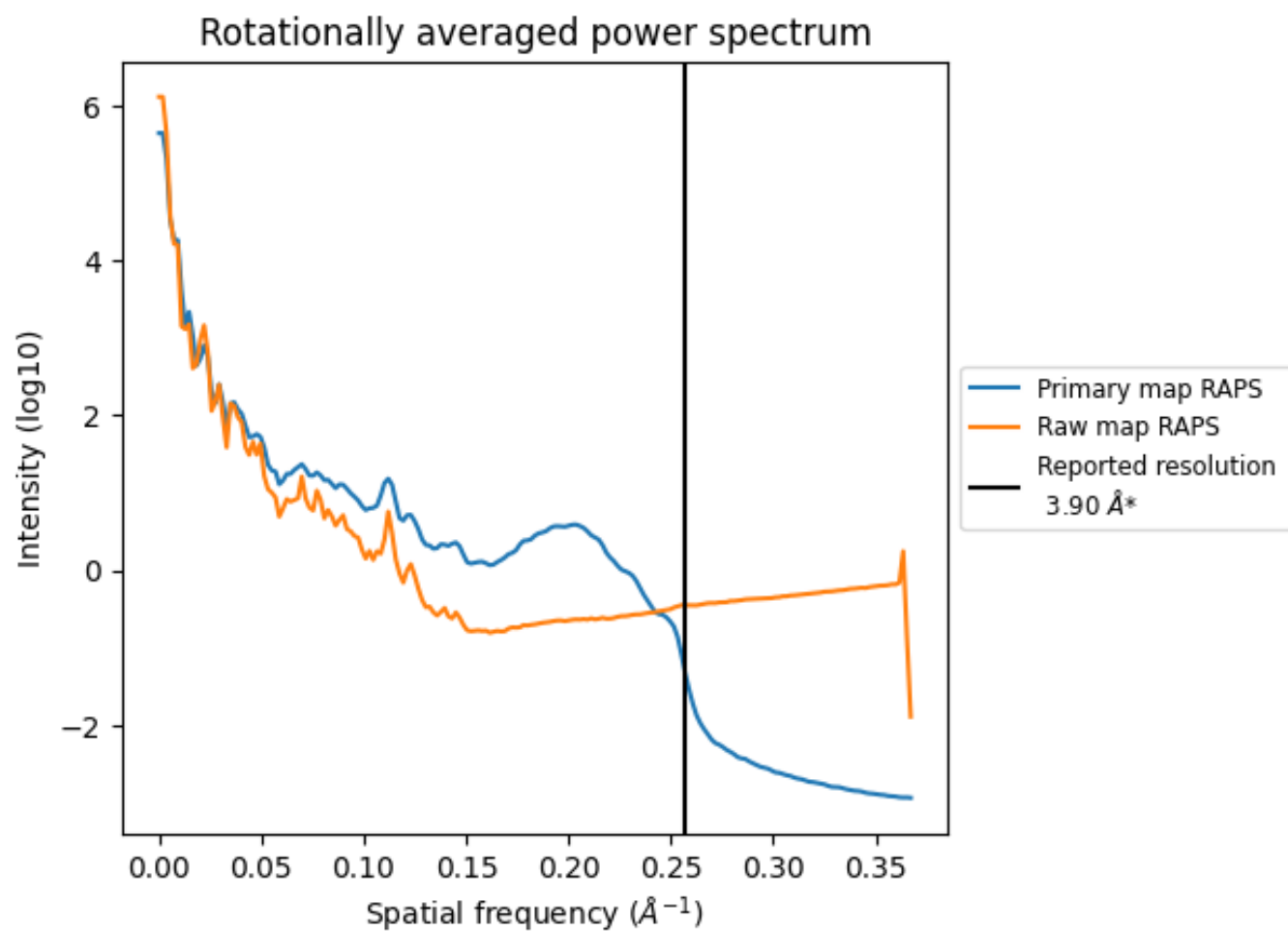
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 904 nm<sup>3</sup>; this corresponds to an approximate mass of 817 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 ⓘ

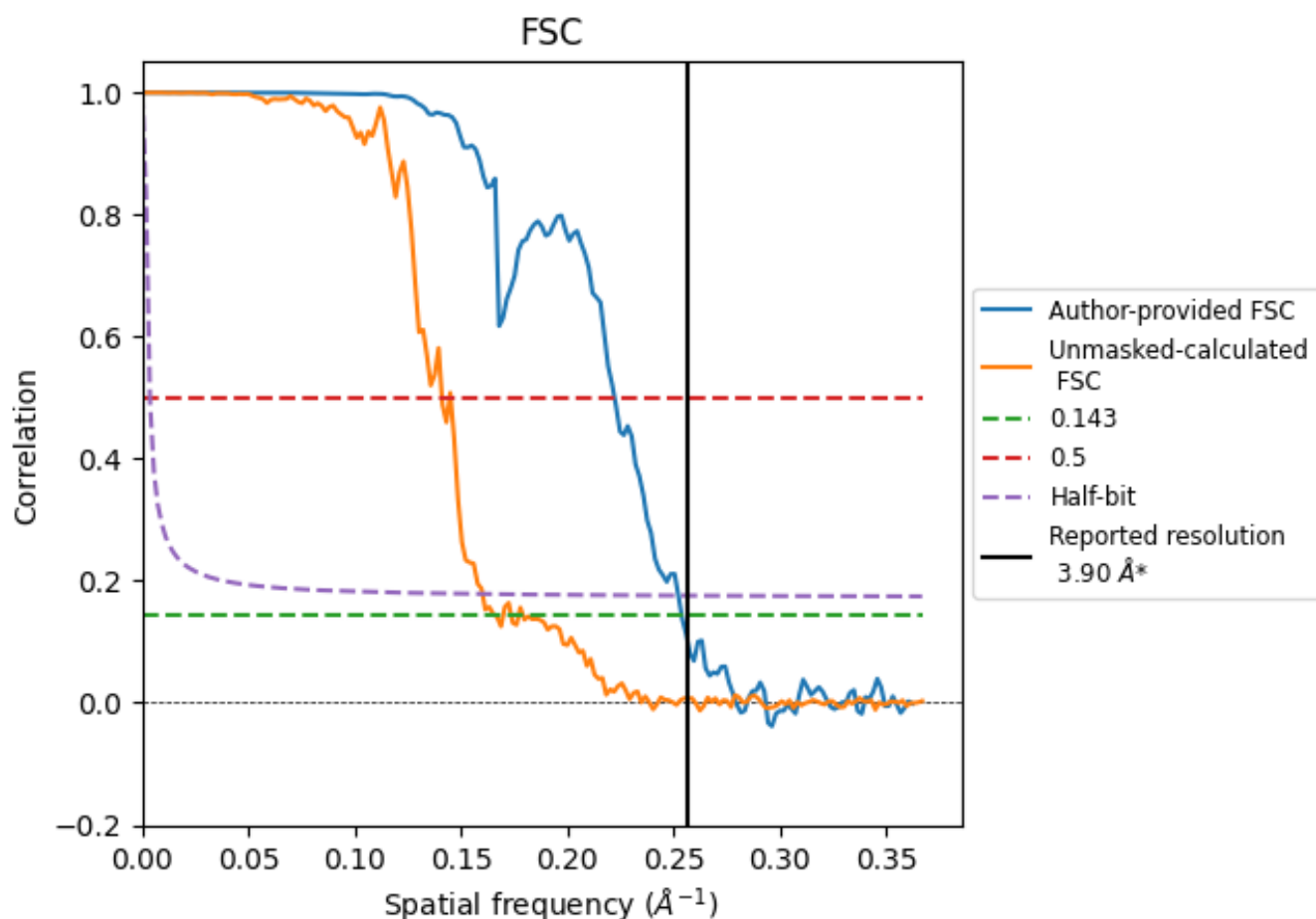


\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 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 0.256  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

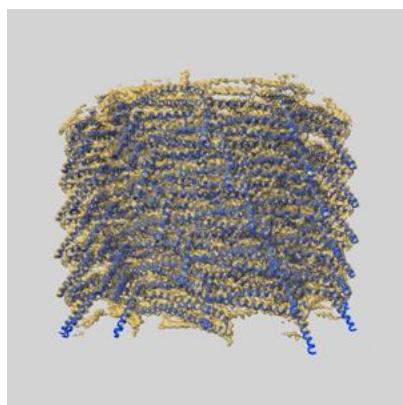
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.90                               | -    | -        |
| Author-provided FSC curve | 3.94                               | 4.50 | 3.96     |
| Unmasked-calculated*      | 6.02                               | 7.09 | 6.24     |

\*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 6.02 differs from the reported value 3.9 by more than 10 %

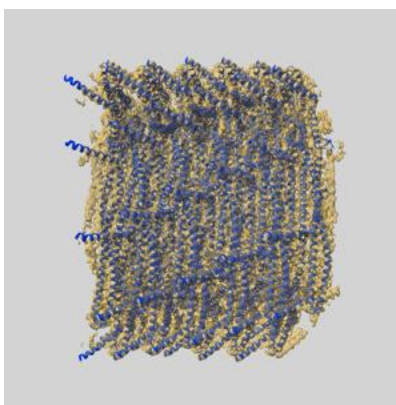
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15491 and PDB model 8AKS. Per-residue inclusion information can be found in section 3 on page 46.

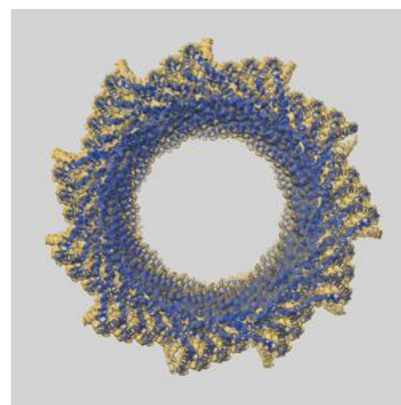
### 9.1 Map-model overlay [i](#)



X



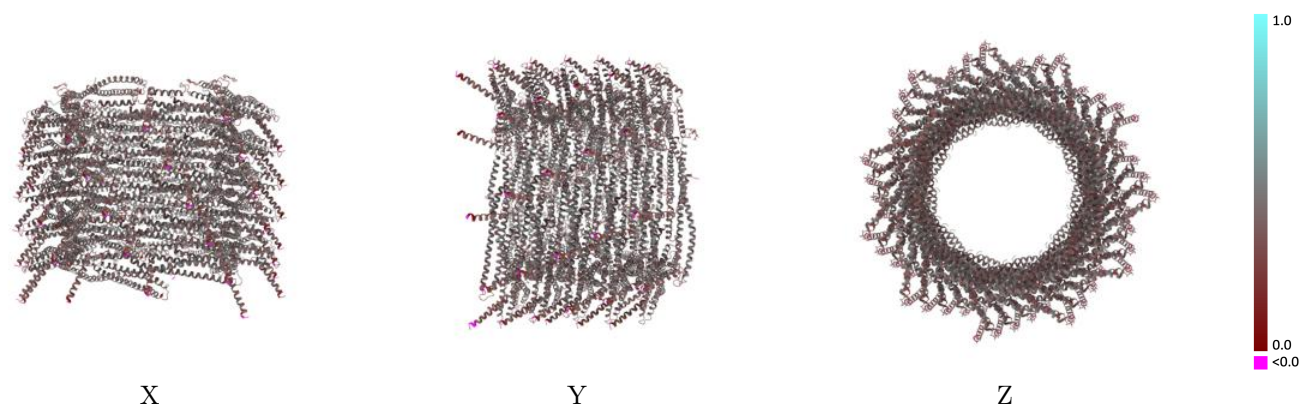
Y



Z

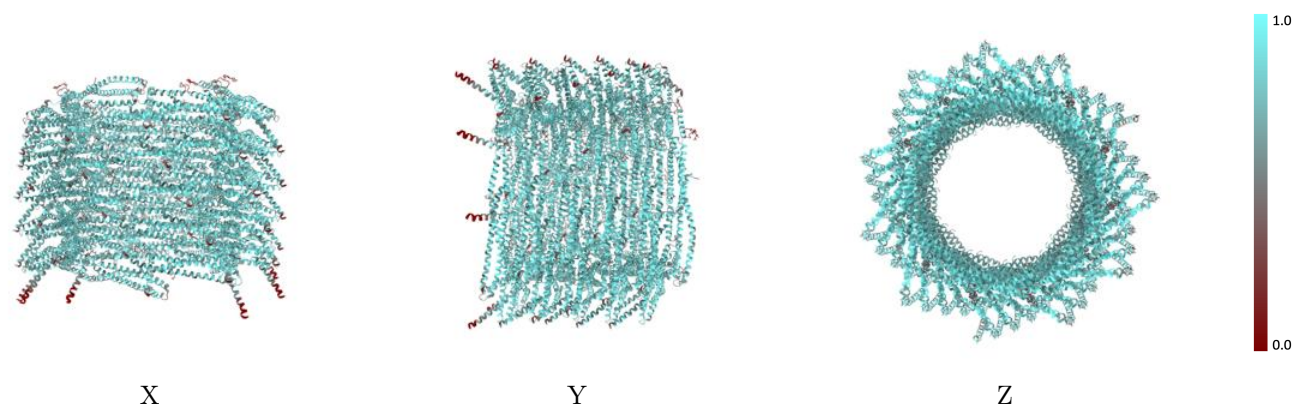
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



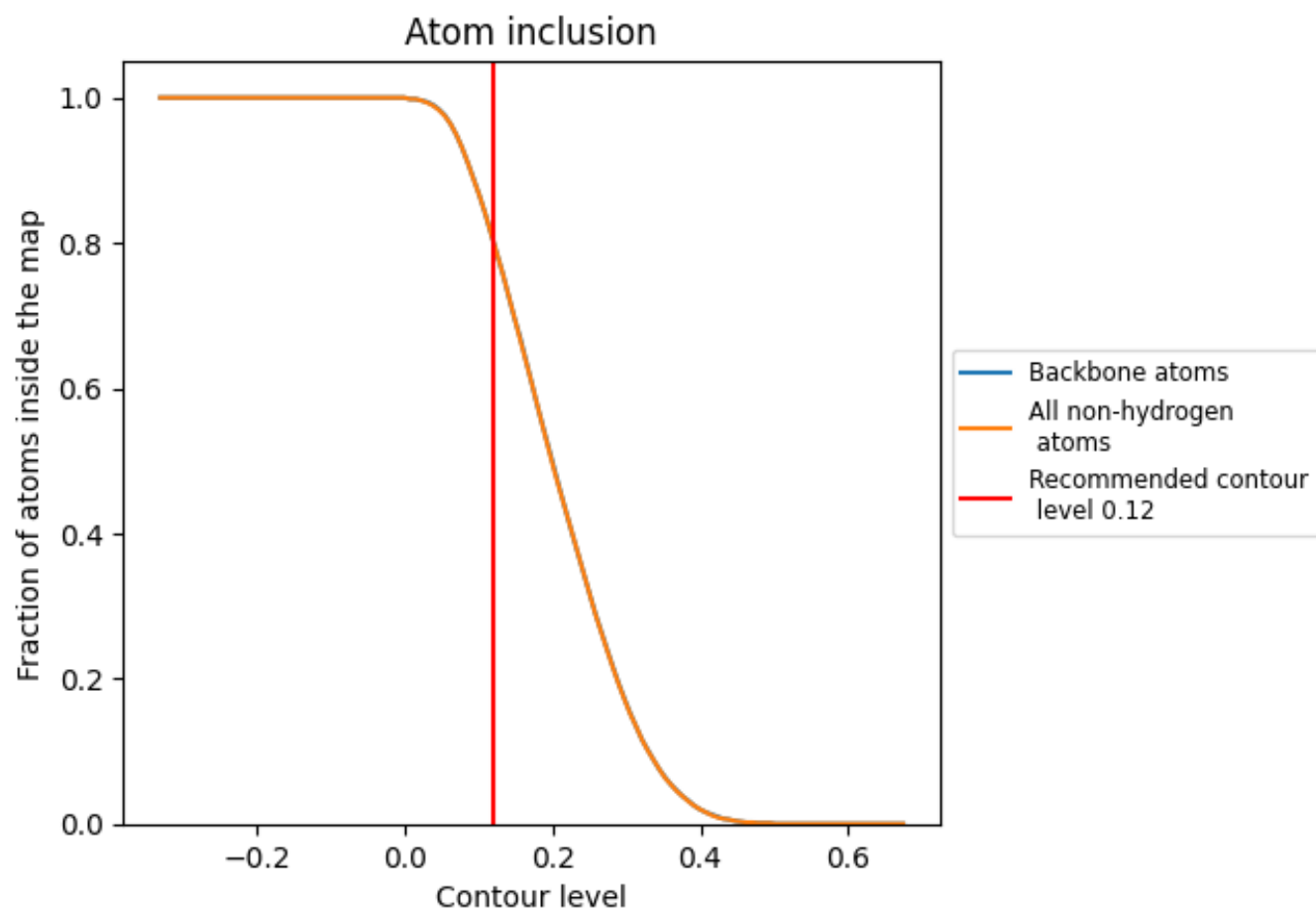
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.12) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8030   |  0.3880   |
| 0     |  0.8010   |  0.3890   |
| 1     |  0.7830   |  0.3900   |
| 2     |  0.7990   |  0.3810   |
| 3     |  0.7760   |  0.3860   |
| 4     |  0.7850   |  0.3940   |
| 5     |  0.7470   |  0.3830   |
| 6     |  0.7170   |  0.3810   |
| 7     |  0.7470   |  0.3910   |
| A     |  0.7300   |  0.3860   |
| B     |  0.7260   |  0.3820   |
| C     |  0.7390   |  0.3870   |
| D     |  0.7720   |  0.3850   |
| E     |  0.7880   |  0.3880   |
| F     |  0.7740  |  0.3880  |
| G     |  0.7830 |  0.3770 |
| H     |  0.8060 |  0.3860 |
| I     |  0.8230 |  0.3980 |
| J     |  0.8270 |  0.3860 |
| K     |  0.8180 |  0.3860 |
| L     |  0.8400 |  0.3940 |
| M     |  0.8270 |  0.3910 |
| N     |  0.8200 |  0.3860 |
| O     |  0.8430 |  0.3890 |
| P     |  0.8330 |  0.3900 |
| Q     |  0.8200 |  0.3920 |
| R     |  0.8370 |  0.3830 |
| S     |  0.8340 |  0.3890 |
| T     |  0.8330 |  0.3950 |
| U     |  0.8340 |  0.3860 |
| V     |  0.8260 |  0.3860 |
| W     |  0.8370 |  0.3950 |
| X     |  0.8310 |  0.3900 |
| Y     |  0.8170 |  0.3880 |
| Z     |  0.8450 |  0.3910 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| a     |  0.8360   |  0.3920   |
| b     |  0.8230   |  0.3910   |
| c     |  0.8470   |  0.3850   |
| d     |  0.8340   |  0.3890   |
| e     |  0.8300   |  0.3950   |
| f     |  0.8340   |  0.3840   |
| g     |  0.8290   |  0.3890   |
| h     |  0.8390   |  0.3950   |
| i     |  0.8310   |  0.3890   |
| j     |  0.8220   |  0.3860   |
| k     |  0.8450   |  0.3920   |
| l     |  0.8330   |  0.3890   |
| m     |  0.8220   |  0.3890   |
| n     |  0.8460   |  0.3830   |
| o     |  0.8370   |  0.3920   |
| p     |  0.8240   |  0.3920   |
| q     |  0.8340   |  0.3820   |
| r     |  0.8280  |  0.3870  |
| s     |  0.8360 |  0.3970 |
| t     |  0.8300 |  0.3880 |
| u     |  0.7040 |  0.3800 |
| v     |  0.8200 |  0.3860 |
| w     |  0.8430 |  0.3910 |
| x     |  0.8310 |  0.3890 |
| y     |  0.8060 |  0.3890 |
| z     |  0.8260 |  0.3850 |