



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 07:15 PM UTC

PDB ID : 6RKE / pdb\_00006rke  
Title : Molybdenum storage protein - P212121, ADP, molybdate  
Authors : Ermler, U.; Bruenle, S.  
Deposited on : 2019-04-30  
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

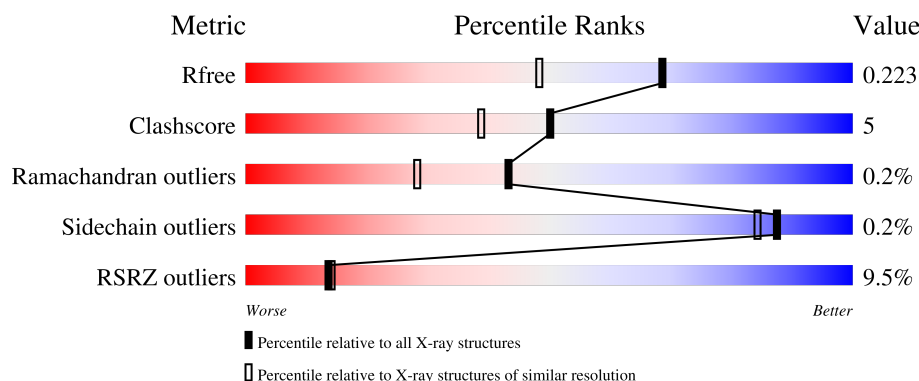
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 5551 (1.70-1.70)                                      |
| Clashscore            | 190562                      | 5924 (1.70-1.70)                                      |
| Ramachandran outliers | 187476                      | 5846 (1.70-1.70)                                      |
| Sidechain outliers    | 187428                      | 5846 (1.70-1.70)                                      |
| RSRZ outliers         | 180081                      | 5554 (1.70-1.70)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                               |
|-----|-------|--------|------------------------------------------------------------------------------------------------|
| 1   | B     | 269    | <div> <div>10%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> </div>             |
| 1   | D     | 269    | <div> <div>11%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> </div>             |
| 1   | F     | 269    | <div> <div>12%</div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>             |
| 1   | H     | 269    | <div> <div>15%</div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </div>              |
| 1   | J     | 269    | <div> <div>12%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div></div> </div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | L     | 269    |                  |
| 2   | A     | 275    |                  |
| 2   | C     | 275    |                  |
| 2   | E     | 275    |                  |
| 2   | G     | 275    |                  |
| 2   | I     | 275    |                  |
| 2   | K     | 275    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res    | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|--------|-----------|----------|---------|------------------|
| 6   | MOO  | B     | 304[A] | -         | -        | X       | -                |
| 6   | MOO  | D     | 303[A] | -         | -        | X       | -                |
| 6   | MOO  | F     | 304[A] | -         | -        | X       | -                |
| 6   | MOO  | H     | 304[A] | -         | -        | X       | -                |
| 6   | MOO  | J     | 304[A] | -         | -        | X       | -                |
| 6   | MOO  | L     | 304[A] | -         | -        | X       | -                |

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 26584 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

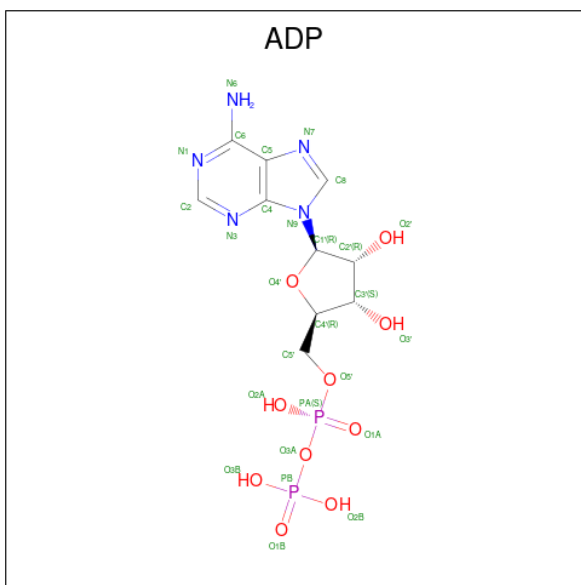
- Molecule 1 is a protein called Molybdenum storage protein subunit beta.

| Mol | Chain | Residues | Atoms         |           |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| 1   | B     | 268      | Total<br>1997 | C<br>1268 | N<br>348 | O<br>373 | S<br>8 | 0       | 5       | 0     |
| 1   | D     | 268      | Total<br>1997 | C<br>1269 | N<br>349 | O<br>371 | S<br>8 | 0       | 4       | 0     |
| 1   | F     | 269      | Total<br>1996 | C<br>1267 | N<br>348 | O<br>373 | S<br>8 | 0       | 4       | 0     |
| 1   | H     | 268      | Total<br>1987 | C<br>1260 | N<br>347 | O<br>372 | S<br>8 | 0       | 3       | 0     |
| 1   | J     | 267      | Total<br>1994 | C<br>1269 | N<br>346 | O<br>371 | S<br>8 | 0       | 6       | 0     |
| 1   | L     | 267      | Total<br>1992 | C<br>1266 | N<br>346 | O<br>372 | S<br>8 | 0       | 6       | 0     |

- Molecule 2 is a protein called Molybdenum storage protein subunit alpha.

| Mol | Chain | Residues | Atoms         |           |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| 2   | A     | 272      | Total<br>2048 | C<br>1292 | N<br>386 | O<br>367 | S<br>3 | 0       | 2       | 0     |
| 2   | C     | 271      | Total<br>2043 | C<br>1289 | N<br>385 | O<br>366 | S<br>3 | 0       | 2       | 0     |
| 2   | E     | 272      | Total<br>2050 | C<br>1293 | N<br>386 | O<br>368 | S<br>3 | 0       | 2       | 0     |
| 2   | G     | 272      | Total<br>2053 | C<br>1295 | N<br>386 | O<br>369 | S<br>3 | 0       | 3       | 0     |
| 2   | I     | 272      | Total<br>2050 | C<br>1293 | N<br>386 | O<br>368 | S<br>3 | 0       | 2       | 0     |
| 2   | K     | 272      | Total<br>2062 | C<br>1301 | N<br>387 | O<br>371 | S<br>3 | 0       | 5       | 0     |

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms       |         |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 3   | B     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 3   | D     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 3   | F     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 3   | H     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 3   | J     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |
| 3   | L     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       | 0       |

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

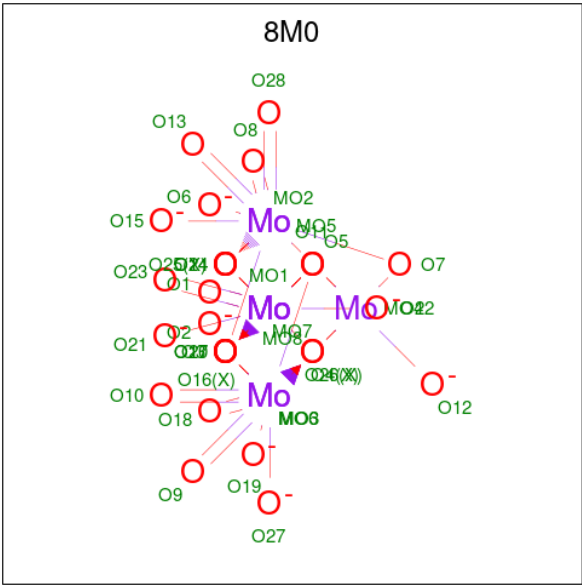
| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4   | B     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 4   | A     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 4   | D     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 4   | C     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 4   | F     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 4   | E     | 1        | Total Mg<br>1 1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | H     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | G     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | J     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | I     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | L     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | K     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 5 is bis(mu4-oxo)-tetrakis(mu3-oxo)-hexakis(mu2-oxo)-hexadeca-oxo-octamolybdenum (VI) (CCD ID: 8M0) (formula: Mo<sub>8</sub>O<sub>28</sub>).



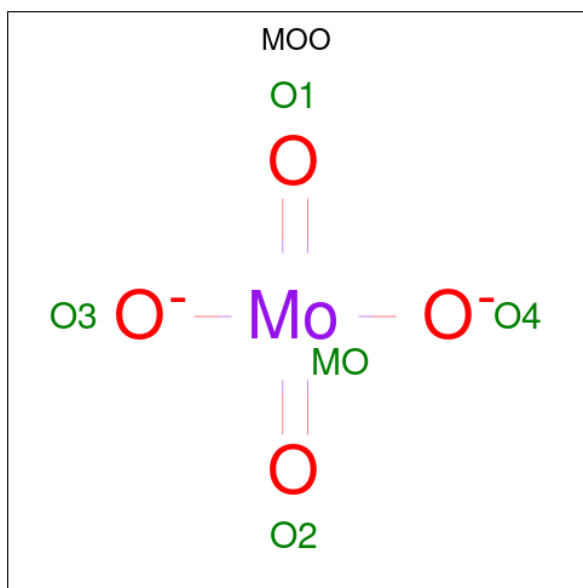
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 5   | B     | 1        | Total | Mo | O  | 0       | 0       |
|     |       |          | 36    | 8  | 28 |         |         |
| 5   | A     | 1        | Total | Mo | O  | 0       | 0       |
|     |       |          | 34    | 8  | 26 |         |         |
| 5   | C     | 1        | Total | Mo | O  | 0       | 0       |
|     |       |          | 36    | 8  | 28 |         |         |
| 5   | C     | 1        | Total | Mo | O  | 0       | 0       |
|     |       |          | 34    | 8  | 26 |         |         |
| 5   | F     | 1        | Total | Mo | O  | 0       | 0       |
|     |       |          | 36    | 8  | 28 |         |         |

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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 5   | E     | 1        | Total | Mo | O  | 0       | 0       |
|     |       |          | 34    | 8  | 26 |         |         |
| 5   | H     | 1        | Total | Mo | O  | 0       | 0       |
|     |       |          | 36    | 8  | 28 |         |         |
| 5   | G     | 1        | Total | Mo | O  | 0       | 0       |
|     |       |          | 34    | 8  | 26 |         |         |
| 5   | J     | 1        | Total | Mo | O  | 0       | 0       |
|     |       |          | 36    | 8  | 28 |         |         |
| 5   | I     | 1        | Total | Mo | O  | 0       | 0       |
|     |       |          | 34    | 8  | 26 |         |         |
| 5   | L     | 1        | Total | Mo | O  | 0       | 0       |
|     |       |          | 36    | 8  | 28 |         |         |
| 5   | K     | 1        | Total | Mo | O  | 0       | 0       |
|     |       |          | 34    | 8  | 26 |         |         |

- Molecule 6 is MOLYBDATE ION (CCD ID: MOO) (formula:  $\text{MoO}_4$ ) (labeled as "Ligand of Interest" by depositor).



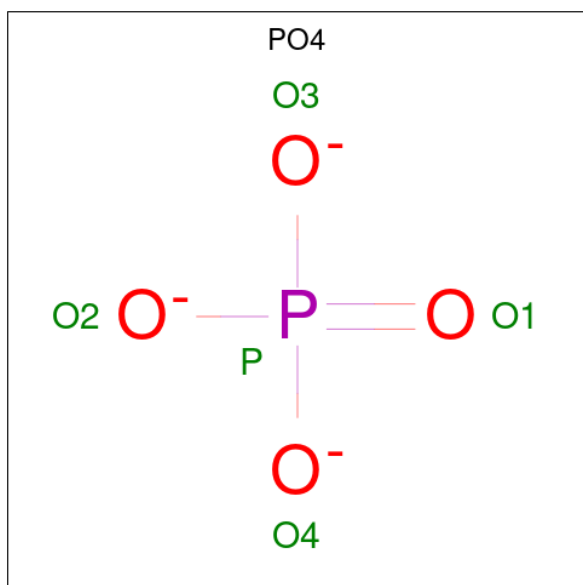
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 6   | B     | 1        | Total | Mo | O | 0       | 1       |
|     |       |          | 5     | 1  | 4 |         |         |
| 6   | D     | 1        | Total | Mo | O | 0       | 1       |
|     |       |          | 5     | 1  | 4 |         |         |
| 6   | F     | 1        | Total | Mo | O | 0       | 1       |
|     |       |          | 5     | 1  | 4 |         |         |
| 6   | H     | 1        | Total | Mo | O | 0       | 1       |
|     |       |          | 5     | 1  | 4 |         |         |

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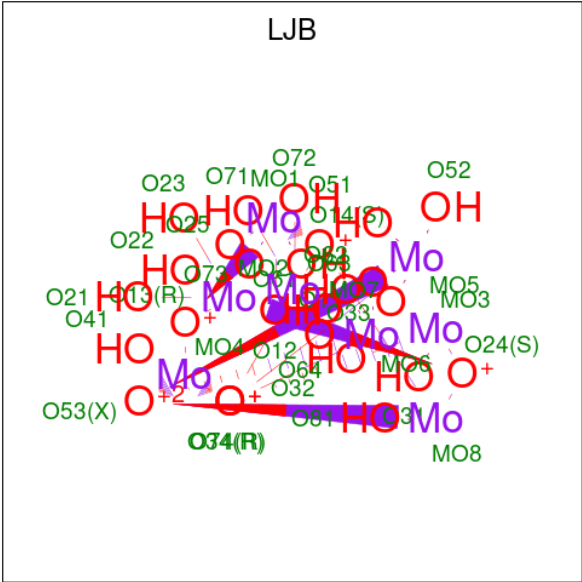
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 6   | J     | 1        | Total | Mo | O | 0       | 1       |
|     |       |          | 5     | 1  | 4 |         |         |
| 6   | L     | 1        | Total | Mo | O | 0       | 1       |
|     |       |          | 5     | 1  | 4 |         |         |

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula:  $O_4P$ ).



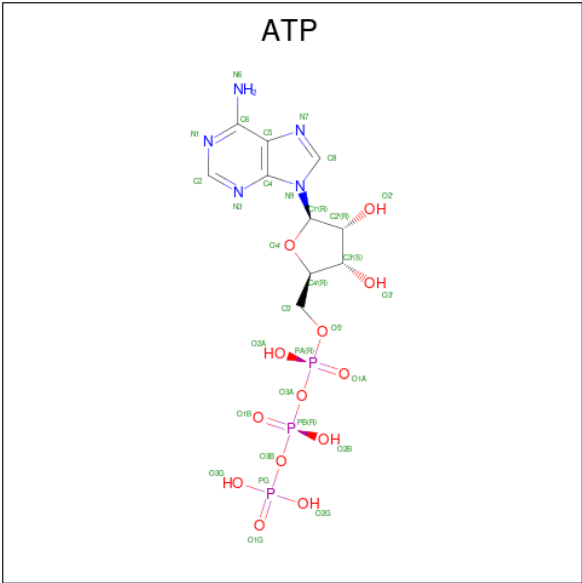
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 7   | B     | 1        | Total | O | P | 0       | 1       |
|     |       |          | 5     | 4 | 1 |         |         |
| 7   | D     | 1        | Total | O | P | 0       | 1       |
|     |       |          | 5     | 4 | 1 |         |         |
| 7   | F     | 1        | Total | O | P | 0       | 1       |
|     |       |          | 5     | 4 | 1 |         |         |
| 7   | H     | 1        | Total | O | P | 0       | 1       |
|     |       |          | 5     | 4 | 1 |         |         |
| 7   | J     | 1        | Total | O | P | 0       | 1       |
|     |       |          | 5     | 4 | 1 |         |         |
| 7   | L     | 1        | Total | O | P | 0       | 1       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 8 is MO(8)-O(26) Cluster (CCD ID: LJB) (formula:  $H_{15}Mo_8O_{26}$ ).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 8   | B     | 1        | Total | Mo | O  | 26      | 0       |
|     |       |          | 34    | 8  | 26 |         |         |
| 8   | L     | 1        | Total | Mo | O  | 26      | 0       |
|     |       |          | 34    | 8  | 26 |         |         |

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



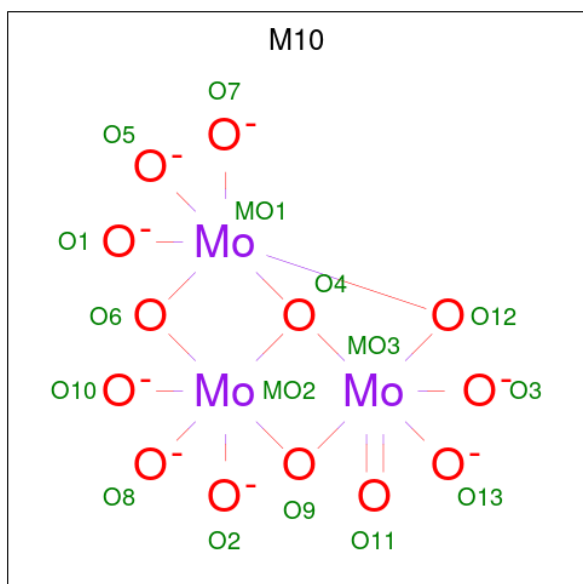
| Mol | Chain | Residues | Atoms       |         |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 9   | A     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>13 | P<br>3 | 0       | 0       |
| 9   | C     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>13 | P<br>3 | 0       | 0       |

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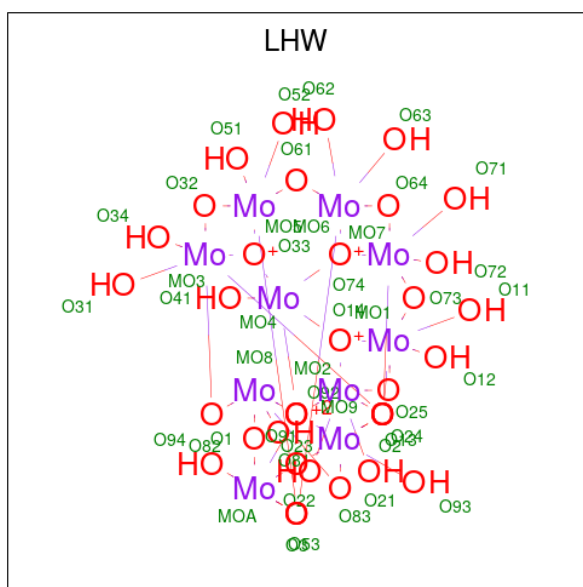
| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 9   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |
| 9   | G     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |
| 9   | I     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |
| 9   | K     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |

- Molecule 10 is (mu3-oxo)-tris(mu2-oxo)-nonakisoxo-trimolybdenum (VI) (CCD ID: M10) (formula:  $\text{Mo}_3\text{O}_{13}$ ).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 10  | A     | 1        | Total | Mo | O  | 0       | 0       |
|     |       |          | 13    | 3  | 10 |         |         |
| 10  | G     | 1        | Total | Mo | O  | 0       | 0       |
|     |       |          | 13    | 3  | 10 |         |         |

- Molecule 11 is MO(10)-O(35) Cluster (CCD ID: LHW) (formula:  $\text{H}_{16}\text{Mo}_{10}\text{O}_{35}$ ).



| Mol | Chain | Residues | Atoms       |          |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|---------|
| 11  | C     | 1        | Total<br>45 | Mo<br>10 | O<br>35 | 35      | 0       |
| 11  | K     | 1        | Total<br>45 | Mo<br>10 | O<br>35 | 34      | 0       |

- Molecule 12 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 12  | B     | 119      | Total O<br>119 119 | 0       | 2       |
| 12  | A     | 162      | Total O<br>162 162 | 0       | 0       |
| 12  | D     | 97       | Total O<br>97 97   | 0       | 2       |
| 12  | C     | 130      | Total O<br>130 130 | 0       | 0       |
| 12  | F     | 98       | Total O<br>98 98   | 0       | 1       |
| 12  | E     | 135      | Total O<br>135 135 | 0       | 0       |
| 12  | H     | 54       | Total O<br>54 54   | 0       | 2       |
| 12  | G     | 118      | Total O<br>118 118 | 0       | 0       |
| 12  | J     | 76       | Total O<br>76 76   | 0       | 0       |
| 12  | I     | 97       | Total O<br>97 97   | 0       | 0       |

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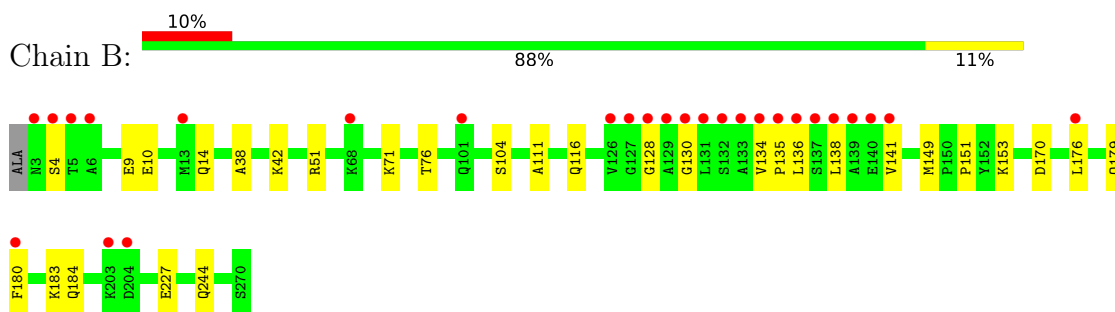
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 12  | L     | 87       | Total<br>87  | O<br>87  | 0       | 1       |
| 12  | K     | 118      | Total<br>118 | O<br>118 | 0       | 0       |

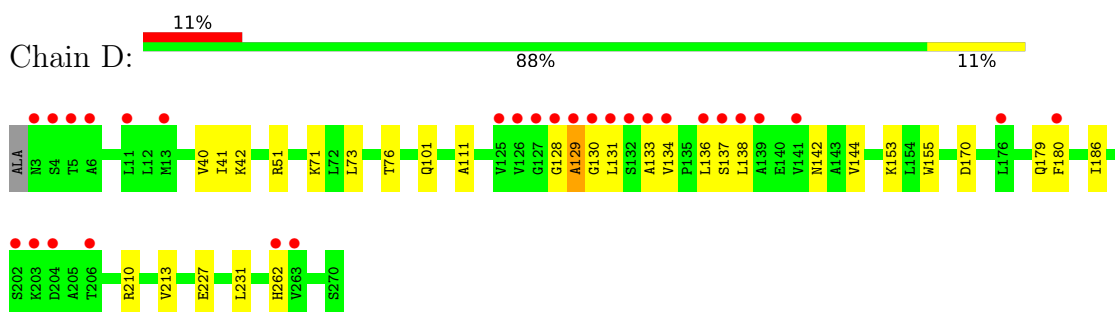
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

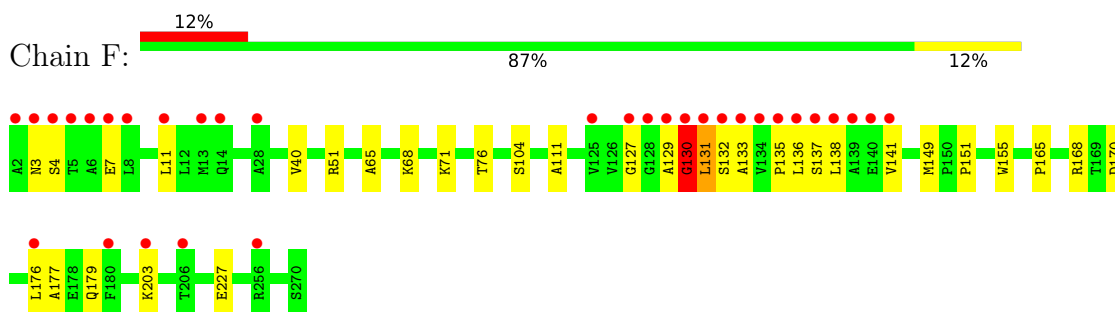
- Molecule 1: Molybdenum storage protein subunit beta



- Molecule 1: Molybdenum storage protein subunit beta

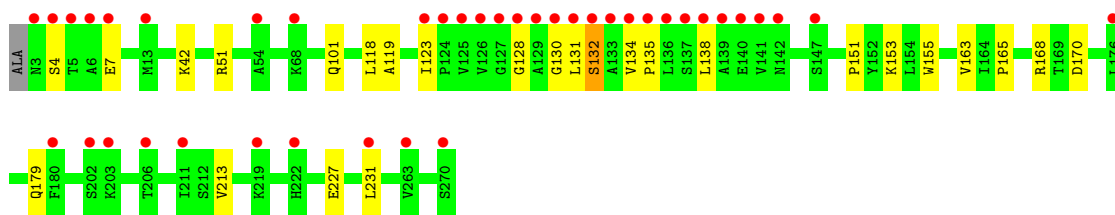


- Molecule 1: Molybdenum storage protein subunit beta

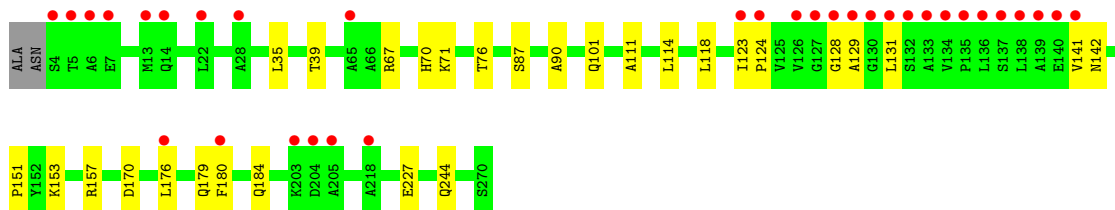
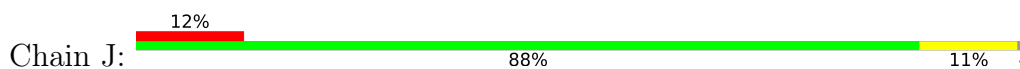


- Molecule 1: Molybdenum storage protein subunit beta

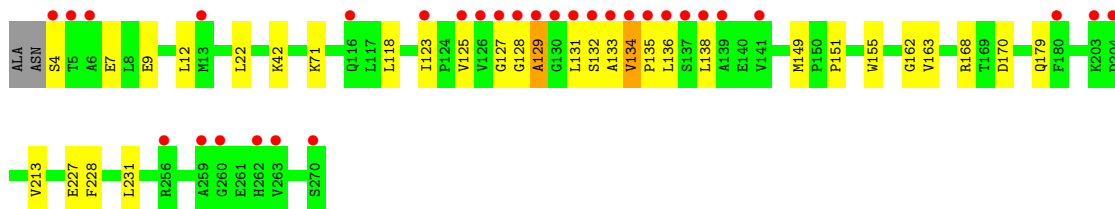
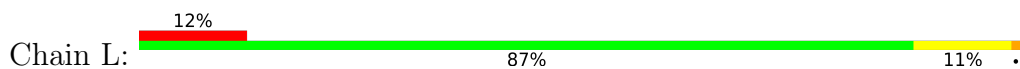




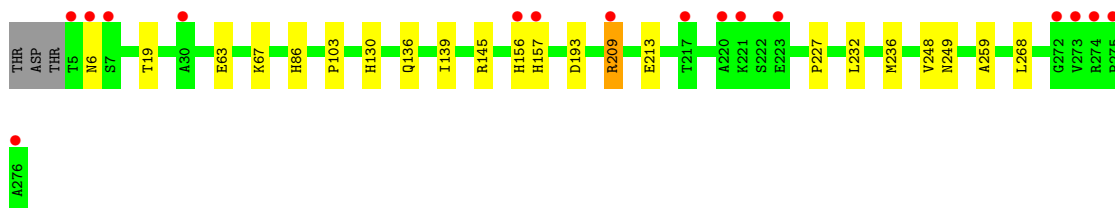
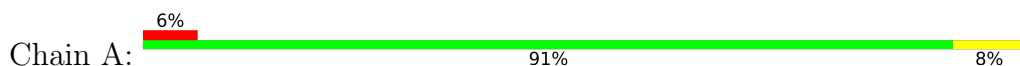
- Molecule 1: Molybdenum storage protein subunit beta



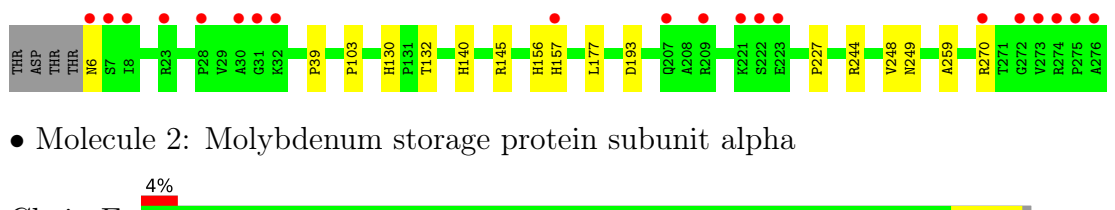
- Molecule 1: Molybdenum storage protein subunit beta



- Molecule 2: Molybdenum storage protein subunit alpha



- Molecule 2: Molybdenum storage protein subunit alpha

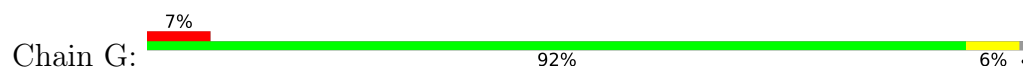


- Molecule 2: Molybdenum storage protein subunit alpha

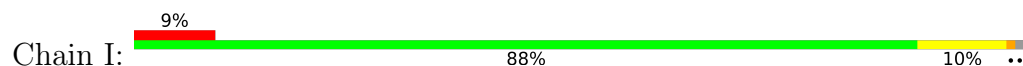




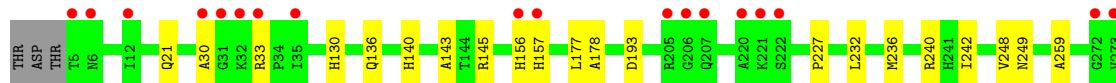
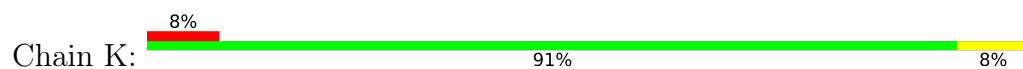
- Molecule 2: Molybdenum storage protein subunit alpha



- Molecule 2: Molybdenum storage protein subunit alpha



- Molecule 2: Molybdenum storage protein subunit alpha



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 128.06Å 148.86Å 183.17Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.49 – 1.70<br>49.49 – 1.70                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.2 (49.49-1.70)<br>97.7 (49.49-1.70)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.30 (at 1.70Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (1.14_3260: ???)                                     | Depositor        |
| R, $R_{free}$                                                           | 0.194 , 0.214<br>0.203 , 0.223                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 19189 reflections (5.03%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 21.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.100                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 32.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 26584                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 27.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, LJB, MOO, LHW, MG, ADP, PO4, 8M0, M10

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   | B     | 0.17         | 0/2048         | 0.36        | 0/2782         |
| 1   | D     | 0.16         | 0/2045         | 0.32        | 0/2777         |
| 1   | F     | 0.27         | 0/2044         | 0.45        | 2/2777 (0.1%)  |
| 1   | H     | 0.26         | 1/2031 (0.0%)  | 0.39        | 0/2759         |
| 1   | J     | 0.22         | 0/2048         | 0.35        | 0/2782         |
| 1   | L     | 0.26         | 1/2046 (0.0%)  | 0.46        | 3/2779 (0.1%)  |
| 2   | A     | 0.16         | 0/2097         | 0.35        | 0/2857         |
| 2   | C     | 0.30         | 0/2092         | 0.40        | 0/2850         |
| 2   | E     | 0.13         | 0/2099         | 0.31        | 0/2860         |
| 2   | G     | 0.20         | 0/2105         | 0.39        | 1/2868 (0.0%)  |
| 2   | I     | 0.22         | 0/2099         | 0.46        | 2/2860 (0.1%)  |
| 2   | K     | 0.16         | 0/2120         | 0.36        | 0/2888         |
| All | All   | 0.22         | 2/24874 (0.0%) | 0.39        | 8/33839 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | F     | 0                   | 2                   |
| 2   | K     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | H     | 132 | SER  | CA-CB | -5.23 | 1.46        | 1.53     |
| 1   | L     | 134 | VAL  | CA-CB | 5.23  | 1.57        | 1.54     |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | G     | 67  | LYS  | CD-CE-NZ | -9.06 | 82.90       | 111.90   |
| 1   | L     | 128 | GLY  | CA-C-N   | 8.85  | 138.43      | 121.54   |
| 1   | L     | 128 | GLY  | C-N-CA   | 8.85  | 138.43      | 121.54   |
| 2   | I     | 274 | ARG  | CB-CA-C  | 6.73  | 119.00      | 108.63   |
| 2   | I     | 274 | ARG  | CB-CG-CD | 6.10  | 125.32      | 111.30   |
| 1   | F     | 131 | LEU  | CA-C-N   | 5.63  | 132.29      | 121.54   |
| 1   | F     | 131 | LEU  | C-N-CA   | 5.63  | 132.29      | 121.54   |
| 1   | L     | 128 | GLY  | O-C-N    | 5.59  | 129.96      | 122.70   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | F     | 130 | GLY  | Mainchain,Peptide |
| 2   | K     | 274 | ARG  | Peptide           |

## 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   | B     | 1997  | 0        | 2058     | 24      | 0            |
| 1   | D     | 1997  | 0        | 2061     | 22      | 0            |
| 1   | F     | 1996  | 0        | 2055     | 38      | 0            |
| 1   | H     | 1987  | 0        | 2043     | 22      | 0            |
| 1   | J     | 1994  | 0        | 2063     | 26      | 0            |
| 1   | L     | 1992  | 0        | 2057     | 28      | 0            |
| 2   | A     | 2048  | 0        | 2105     | 18      | 0            |
| 2   | C     | 2043  | 0        | 2103     | 19      | 0            |
| 2   | E     | 2050  | 0        | 2110     | 19      | 0            |
| 2   | G     | 2053  | 0        | 2115     | 16      | 0            |
| 2   | I     | 2050  | 0        | 2110     | 21      | 0            |
| 2   | K     | 2062  | 0        | 2128     | 25      | 0            |
| 3   | B     | 27    | 0        | 12       | 1       | 0            |
| 3   | D     | 27    | 0        | 12       | 0       | 0            |
| 3   | F     | 27    | 0        | 12       | 0       | 0            |
| 3   | H     | 27    | 0        | 12       | 0       | 0            |
| 3   | J     | 27    | 0        | 12       | 0       | 0            |
| 3   | L     | 27    | 0        | 12       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | C     | 1     | 0        | 0        | 0       | 0            |
| 4   | D     | 1     | 0        | 0        | 0       | 0            |
| 4   | E     | 1     | 0        | 0        | 0       | 0            |
| 4   | F     | 1     | 0        | 0        | 0       | 0            |
| 4   | G     | 1     | 0        | 0        | 0       | 0            |
| 4   | H     | 1     | 0        | 0        | 0       | 0            |
| 4   | I     | 1     | 0        | 0        | 0       | 0            |
| 4   | J     | 1     | 0        | 0        | 0       | 0            |
| 4   | K     | 1     | 0        | 0        | 0       | 0            |
| 4   | L     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 34    | 0        | 0        | 1       | 0            |
| 5   | B     | 36    | 0        | 0        | 4       | 0            |
| 5   | C     | 70    | 0        | 0        | 4       | 0            |
| 5   | E     | 34    | 0        | 0        | 1       | 0            |
| 5   | F     | 36    | 0        | 0        | 6       | 0            |
| 5   | G     | 34    | 0        | 0        | 1       | 0            |
| 5   | H     | 36    | 0        | 0        | 2       | 0            |
| 5   | I     | 34    | 0        | 0        | 1       | 0            |
| 5   | J     | 36    | 0        | 0        | 2       | 0            |
| 5   | K     | 34    | 0        | 0        | 2       | 0            |
| 5   | L     | 36    | 0        | 0        | 5       | 0            |
| 6   | B     | 5     | 0        | 0        | 4       | 0            |
| 6   | D     | 5     | 0        | 0        | 4       | 0            |
| 6   | F     | 5     | 0        | 0        | 4       | 0            |
| 6   | H     | 5     | 0        | 0        | 4       | 0            |
| 6   | J     | 5     | 0        | 0        | 4       | 0            |
| 6   | L     | 5     | 0        | 0        | 4       | 0            |
| 7   | B     | 5     | 0        | 0        | 0       | 0            |
| 7   | D     | 5     | 0        | 0        | 0       | 0            |
| 7   | F     | 5     | 0        | 0        | 0       | 0            |
| 7   | H     | 5     | 0        | 0        | 0       | 0            |
| 7   | J     | 5     | 0        | 0        | 0       | 0            |
| 7   | L     | 5     | 0        | 0        | 0       | 0            |
| 8   | B     | 34    | 0        | 0        | 0       | 0            |
| 8   | L     | 34    | 0        | 0        | 0       | 0            |
| 9   | A     | 31    | 0        | 12       | 1       | 0            |
| 9   | C     | 31    | 0        | 12       | 1       | 0            |
| 9   | E     | 31    | 0        | 12       | 2       | 0            |
| 9   | G     | 31    | 0        | 12       | 2       | 0            |
| 9   | I     | 31    | 0        | 12       | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | K     | 31    | 0        | 12       | 1       | 0            |
| 10  | A     | 13    | 0        | 0        | 3       | 0            |
| 10  | G     | 13    | 0        | 0        | 3       | 0            |
| 11  | C     | 45    | 0        | 0        | 0       | 0            |
| 11  | K     | 45    | 0        | 0        | 0       | 0            |
| 12  | A     | 162   | 0        | 0        | 1       | 0            |
| 12  | B     | 119   | 0        | 0        | 1       | 0            |
| 12  | C     | 130   | 0        | 0        | 0       | 0            |
| 12  | D     | 97    | 0        | 0        | 1       | 0            |
| 12  | E     | 135   | 0        | 0        | 0       | 0            |
| 12  | F     | 98    | 0        | 0        | 0       | 0            |
| 12  | G     | 118   | 0        | 0        | 4       | 0            |
| 12  | H     | 54    | 0        | 0        | 0       | 0            |
| 12  | I     | 97    | 0        | 0        | 0       | 0            |
| 12  | J     | 76    | 0        | 0        | 3       | 0            |
| 12  | K     | 118   | 0        | 0        | 3       | 0            |
| 12  | L     | 87    | 0        | 0        | 0       | 0            |
| All | All   | 26584 | 0        | 25152    | 265     | 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 5.

All (265) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:204:ASP:HB3  | 2:I:207:GLN:HE21 | 1.12                     | 1.08              |
| 2:I:202:GLY:O    | 2:I:205:ARG:HG2  | 1.67                     | 0.95              |
| 2:G:219:LEU:O    | 2:G:222:SER:OG   | 1.93                     | 0.86              |
| 1:H:131:LEU:HD11 | 1:L:125:VAL:O    | 1.75                     | 0.85              |
| 2:K:21:GLN:O     | 12:K:401:HOH:O   | 1.95                     | 0.85              |
| 2:I:202:GLY:O    | 2:I:205:ARG:CG   | 2.25                     | 0.84              |
| 1:H:101:GLN:HG2  | 1:H:153:LYS:HD2  | 1.59                     | 0.84              |
| 2:I:204:ASP:HB3  | 2:I:207:GLN:NE2  | 1.92                     | 0.81              |
| 1:L:179:GLN:HG2  | 2:K:157:HIS:HB3  | 1.65                     | 0.78              |
| 1:H:179:GLN:HG2  | 2:G:157:HIS:HB3  | 1.67                     | 0.77              |
| 1:F:179:GLN:HG2  | 2:E:157:HIS:HB3  | 1.66                     | 0.76              |
| 1:H:131:LEU:CD1  | 1:L:125:VAL:O    | 2.33                     | 0.76              |
| 1:F:130:GLY:O    | 1:F:131:LEU:HG   | 1.86                     | 0.75              |
| 1:J:179:GLN:HG2  | 2:I:157:HIS:HB3  | 1.67                     | 0.75              |
| 1:J:129:ALA:HA   | 5:J:302:8M0:O22  | 1.87                     | 0.74              |
| 1:J:35:LEU:HD11  | 1:J:131:LEU:HD11 | 1.69                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:73:LEU:HD21   | 1:D:136:LEU:HD11  | 1.69                     | 0.74              |
| 1:L:129:ALA:HB2   | 5:L:303:8M0:O22   | 1.89                     | 0.73              |
| 1:F:130:GLY:HA2   | 2:E:157:HIS:NE2   | 2.07                     | 0.70              |
| 2:C:39:PRO:HG3    | 12:G:406:HOH:O    | 1.94                     | 0.68              |
| 1:B:179:GLN:HG2   | 2:A:157:HIS:HB3   | 1.76                     | 0.68              |
| 1:J:131:LEU:HD13  | 1:J:180:PHE:CE1   | 2.29                     | 0.67              |
| 1:D:179:GLN:HG2   | 2:C:157:HIS:HB3   | 1.78                     | 0.66              |
| 2:K:274:ARG:HH21  | 2:K:274:ARG:HG3   | 1.61                     | 0.66              |
| 1:F:130:GLY:C     | 1:F:131:LEU:HG    | 2.22                     | 0.65              |
| 1:F:71:LYS:NZ     | 1:F:136:LEU:O     | 2.25                     | 0.64              |
| 1:J:131:LEU:HD13  | 1:J:180:PHE:CZ    | 2.33                     | 0.64              |
| 6:B:304[A]:MOO:MO | 6:B:304[A]:MOO:O1 | 1.70                     | 0.63              |
| 1:B:51:ARG:NH1    | 2:A:6:ASN:O       | 2.32                     | 0.63              |
| 6:B:304[A]:MOO:MO | 6:B:304[A]:MOO:O3 | 1.70                     | 0.63              |
| 6:D:303[A]:MOO:MO | 6:D:303[A]:MOO:O1 | 1.70                     | 0.63              |
| 6:J:304[A]:MOO:O3 | 6:J:304[A]:MOO:MO | 1.70                     | 0.62              |
| 6:L:304[A]:MOO:O3 | 6:L:304[A]:MOO:MO | 1.70                     | 0.62              |
| 6:L:304[A]:MOO:MO | 6:L:304[A]:MOO:O1 | 1.70                     | 0.62              |
| 6:J:304[A]:MOO:MO | 6:J:304[A]:MOO:O1 | 1.70                     | 0.62              |
| 6:F:304[A]:MOO:O1 | 6:F:304[A]:MOO:MO | 1.70                     | 0.62              |
| 6:H:304[A]:MOO:O3 | 6:H:304[A]:MOO:MO | 1.70                     | 0.62              |
| 6:D:303[A]:MOO:MO | 6:D:303[A]:MOO:O3 | 1.70                     | 0.62              |
| 6:H:304[A]:MOO:MO | 6:H:304[A]:MOO:O4 | 1.71                     | 0.62              |
| 2:K:33:ARG:HH12   | 2:K:274:ARG:HH12  | 1.46                     | 0.62              |
| 6:J:304[A]:MOO:MO | 6:J:304[A]:MOO:O4 | 1.72                     | 0.61              |
| 1:J:244:GLN:NE2   | 12:J:401:HOH:O    | 2.23                     | 0.61              |
| 1:B:104[B]:SER:HA | 1:B:149:MET:HG3   | 1.83                     | 0.61              |
| 6:H:304[A]:MOO:MO | 6:H:304[A]:MOO:O1 | 1.70                     | 0.61              |
| 1:B:104[A]:SER:HA | 1:B:149:MET:HG3   | 1.83                     | 0.61              |
| 6:F:304[A]:MOO:MO | 6:F:304[A]:MOO:O2 | 1.72                     | 0.61              |
| 6:D:303[A]:MOO:MO | 6:D:303[A]:MOO:O2 | 1.72                     | 0.61              |
| 6:F:304[A]:MOO:MO | 6:F:304[A]:MOO:O3 | 1.70                     | 0.61              |
| 10:G:304:M10:O2   | 10:G:304:M10:MO2  | 1.72                     | 0.61              |
| 6:F:304[A]:MOO:MO | 6:F:304[A]:MOO:O4 | 1.71                     | 0.61              |
| 10:G:304:M10:O1   | 10:G:304:M10:MO1  | 1.72                     | 0.61              |
| 10:A:304:M10:O1   | 10:A:304:M10:MO1  | 1.72                     | 0.61              |
| 2:C:39:PRO:CG     | 12:G:406:HOH:O    | 2.47                     | 0.61              |
| 10:G:304:M10:O3   | 10:G:304:M10:MO3  | 1.72                     | 0.60              |
| 6:B:304[A]:MOO:MO | 6:B:304[A]:MOO:O2 | 1.72                     | 0.60              |
| 1:F:129:ALA:O     | 1:F:131:LEU:HB2   | 2.01                     | 0.60              |
| 2:I:130:HIS:HB2   | 5:I:303:8M0:O21   | 2.02                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:176:LEU:HD11  | 5:B:303:8M0:O13   | 2.01                     | 0.60              |
| 6:L:304[A]:MOO:MO | 6:L:304[A]:MOO:O4 | 1.72                     | 0.60              |
| 6:L:304[A]:MOO:MO | 6:L:304[A]:MOO:O2 | 1.72                     | 0.60              |
| 1:F:176:LEU:HD11  | 5:F:303:8M0:O13   | 2.02                     | 0.60              |
| 1:L:151:PRO:HB3   | 5:L:303:8M0:O4    | 2.02                     | 0.60              |
| 6:D:303[A]:MOO:MO | 6:D:303[A]:MOO:O4 | 1.72                     | 0.59              |
| 6:B:304[A]:MOO:MO | 6:B:304[A]:MOO:O4 | 1.72                     | 0.59              |
| 6:H:304[A]:MOO:MO | 6:H:304[A]:MOO:O2 | 1.72                     | 0.59              |
| 10:A:304:M10:O2   | 10:A:304:M10:MO2  | 1.72                     | 0.59              |
| 1:B:151:PRO:HB3   | 5:B:303:8M0:O4    | 2.03                     | 0.59              |
| 10:A:304:M10:MO3  | 10:A:304:M10:O13  | 1.72                     | 0.59              |
| 12:D:409:HOH:O    | 1:F:131:LEU:CD2   | 2.50                     | 0.59              |
| 6:J:304[A]:MOO:MO | 6:J:304[A]:MOO:O2 | 1.72                     | 0.59              |
| 1:F:129:ALA:HA    | 5:F:303:8M0:O22   | 2.02                     | 0.58              |
| 2:C:244:ARG:HH21  | 2:C:270:ARG:HH12  | 1.51                     | 0.58              |
| 1:F:127:GLY:HA2   | 5:F:303:8M0:O17   | 2.04                     | 0.57              |
| 1:H:151:PRO:HB3   | 5:H:303:8M0:O4    | 2.04                     | 0.57              |
| 1:B:71:LYS:HG2    | 1:B:136:LEU:HD22  | 1.86                     | 0.57              |
| 1:F:129:ALA:O     | 1:F:131:LEU:N     | 2.37                     | 0.57              |
| 2:K:130:HIS:HB2   | 5:K:303:8M0:O21   | 2.05                     | 0.56              |
| 1:D:210:ARG:NH2   | 1:D:262:HIS:CE1   | 2.73                     | 0.56              |
| 1:J:71:LYS:NZ     | 1:J:142:ASN:OD1   | 2.39                     | 0.56              |
| 1:D:170:ASP:HB2   | 1:D:227:GLU:CD    | 2.31                     | 0.56              |
| 1:D:138:LEU:HD13  | 1:F:138:LEU:HD21  | 1.88                     | 0.56              |
| 1:F:65:ALA:O      | 1:F:68:LYS:HE2    | 2.07                     | 0.55              |
| 5:B:303:8M0:O15   | 2:A:157:HIS:HD2   | 1.89                     | 0.55              |
| 1:H:138:LEU:HD11  | 1:L:138:LEU:HD13  | 1.87                     | 0.55              |
| 1:F:130:GLY:CA    | 2:E:157:HIS:NE2   | 2.68                     | 0.55              |
| 1:H:119:ALA:CB    | 1:J:131:LEU:HD23  | 2.36                     | 0.55              |
| 1:F:130:GLY:N     | 2:E:157:HIS:NE2   | 2.54                     | 0.55              |
| 5:L:303:8M0:O24   | 2:K:156:HIS:ND1   | 2.26                     | 0.55              |
| 2:A:103:PRO:HB3   | 2:A:156:HIS:HD2   | 1.72                     | 0.55              |
| 1:H:132:SER:C     | 1:H:135:PRO:HD2   | 2.33                     | 0.54              |
| 2:C:130:HIS:HB2   | 5:C:304:8M0:O21   | 2.08                     | 0.54              |
| 1:L:4:SER:OG      | 1:L:7:GLU:CB      | 2.55                     | 0.54              |
| 2:I:227:PRO:HD3   | 9:I:301:ATP:C6    | 2.43                     | 0.54              |
| 2:E:46:ILE:HD12   | 2:E:61:LEU:HD21   | 1.89                     | 0.54              |
| 1:F:151:PRO:HB3   | 5:F:303:8M0:O4    | 2.07                     | 0.54              |
| 2:G:67:LYS:NZ     | 12:G:406:HOH:O    | 2.41                     | 0.54              |
| 5:B:303:8M0:O13   | 2:A:157:HIS:HB2   | 2.09                     | 0.53              |
| 1:B:130:GLY:HA3   | 1:B:180:PHE:CE2   | 2.43                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:H:119:ALA:HB1   | 1:J:131:LEU:HD23   | 1.91                     | 0.53              |
| 2:A:130:HIS:HB2   | 5:A:303:8M0:O21    | 2.09                     | 0.53              |
| 1:D:101:GLN:HG2   | 1:D:153[B]:LYS:HD2 | 1.89                     | 0.53              |
| 1:D:129:ALA:HA    | 1:D:144:VAL:HG21   | 1.89                     | 0.53              |
| 1:F:51:ARG:NH1    | 2:E:6:ASN:O        | 2.37                     | 0.53              |
| 1:D:40:VAL:HG22   | 1:D:73:LEU:HB2     | 1.91                     | 0.53              |
| 1:F:127:GLY:HA3   | 5:F:303:8M0:O18    | 2.09                     | 0.53              |
| 1:B:135:PRO:HG3   | 1:D:134:VAL:HG21   | 1.91                     | 0.52              |
| 1:B:116:GLN:HG2   | 1:D:131:LEU:HD21   | 1.91                     | 0.52              |
| 1:J:101:GLN:OE1   | 1:J:153:LYS:HE3    | 2.09                     | 0.52              |
| 1:J:151:PRO:HB3   | 5:J:302:8M0:O4     | 2.10                     | 0.52              |
| 2:G:130:HIS:HB2   | 5:G:303:8M0:O21    | 2.09                     | 0.52              |
| 1:L:170:ASP:HB2   | 1:L:227:GLU:CD     | 2.34                     | 0.51              |
| 1:F:133:ALA:O     | 1:F:137:SER:HB3    | 2.11                     | 0.51              |
| 1:J:124:PRO:HB3   | 1:L:133:ALA:HB3    | 1.93                     | 0.51              |
| 2:K:227:PRO:HD3   | 9:K:301:ATP:C6     | 2.46                     | 0.51              |
| 2:C:157:HIS:HD2   | 5:C:301:8M0:O15    | 1.94                     | 0.51              |
| 2:C:244:ARG:HH21  | 2:C:270:ARG:NH1    | 2.09                     | 0.51              |
| 1:F:4:SER:OG      | 1:F:7:GLU:HB2      | 2.10                     | 0.51              |
| 1:F:170:ASP:HB2   | 1:F:227:GLU:CD     | 2.35                     | 0.51              |
| 1:D:51:ARG:NH1    | 2:C:6:ASN:O        | 2.39                     | 0.51              |
| 2:I:136:GLN:O     | 2:I:140:HIS:ND1    | 2.39                     | 0.51              |
| 1:L:132:SER:O     | 1:L:135:PRO:HD2    | 2.10                     | 0.51              |
| 1:F:104[B]:SER:HA | 1:F:149:MET:HG3    | 1.94                     | 0.50              |
| 2:G:227:PRO:HD3   | 9:G:301:ATP:C6     | 2.45                     | 0.50              |
| 2:E:130:HIS:HB2   | 5:E:303:8M0:O21    | 2.11                     | 0.50              |
| 5:L:303:8M0:O1    | 2:K:156:HIS:CE1    | 2.65                     | 0.50              |
| 1:J:170:ASP:HB2   | 1:J:227:GLU:CD     | 2.37                     | 0.50              |
| 1:F:135:PRO:HB3   | 1:F:141:VAL:HG11   | 1.93                     | 0.50              |
| 1:F:104[A]:SER:HA | 1:F:149:MET:HG3    | 1.94                     | 0.50              |
| 1:J:87:SER:HB3    | 2:I:14:PRO:HG2     | 1.92                     | 0.50              |
| 2:A:136:GLN:NE2   | 12:A:405:HOH:O     | 2.45                     | 0.49              |
| 1:D:210:ARG:NH2   | 1:D:262:HIS:HE1    | 2.10                     | 0.49              |
| 1:H:170:ASP:HB2   | 1:H:227:GLU:CD     | 2.37                     | 0.49              |
| 2:A:227:PRO:HD3   | 9:A:301:ATP:C6     | 2.48                     | 0.49              |
| 1:B:138:LEU:HD13  | 1:D:138:LEU:HD21   | 1.96                     | 0.48              |
| 2:A:213:GLU:HG3   | 2:A:268:LEU:HB2    | 1.95                     | 0.48              |
| 1:F:7:GLU:O       | 1:F:11:LEU:HG      | 2.13                     | 0.48              |
| 2:E:227:PRO:HD3   | 9:E:301:ATP:C6     | 2.49                     | 0.48              |
| 1:F:203:LYS:CD    | 1:F:203:LYS:H      | 2.27                     | 0.48              |
| 1:L:127:GLY:HA2   | 5:L:303:8M0:O17    | 2.13                     | 0.48              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:K:274:ARG:HB2     | 2:K:275:PRO:HD3     | 1.95                     | 0.48              |
| 2:C:157:HIS:HB2     | 5:C:301:8M0:O13     | 2.14                     | 0.47              |
| 2:K:232:LEU:HD11    | 2:K:236:MET:HE3     | 1.96                     | 0.47              |
| 2:A:145[B]:ARG:HH12 | 2:I:145[B]:ARG:HH12 | 1.62                     | 0.47              |
| 1:B:135:PRO:HB3     | 1:B:141:VAL:HG11    | 1.95                     | 0.47              |
| 1:B:170:ASP:HB2     | 1:B:227:GLU:CD      | 2.39                     | 0.47              |
| 5:F:303:8M0:O24     | 2:E:156:HIS:ND1     | 2.43                     | 0.47              |
| 1:H:128:GLY:C       | 1:H:130:GLY:H       | 2.22                     | 0.47              |
| 2:E:145[B]:ARG:HH12 | 2:K:145[B]:ARG:HH12 | 1.63                     | 0.47              |
| 1:H:4:SER:HB3       | 1:H:7:GLU:HB3       | 1.95                     | 0.47              |
| 1:J:70:HIS:HD2      | 12:J:410:HOH:O      | 1.97                     | 0.47              |
| 1:B:104[A]:SER:OG   | 1:B:153:LYS:HE3     | 2.14                     | 0.47              |
| 2:I:103:PRO:HB3     | 2:I:156:HIS:HD2     | 1.80                     | 0.47              |
| 2:C:156:HIS:ND1     | 5:C:301:8M0:O24     | 2.47                     | 0.47              |
| 1:B:183:LYS:O       | 1:B:184:GLN:HG3     | 2.15                     | 0.46              |
| 2:E:248:VAL:HG11    | 2:E:259:ALA:HB2     | 1.98                     | 0.46              |
| 1:H:213:VAL:HG13    | 1:H:231:LEU:HB3     | 1.97                     | 0.46              |
| 2:C:103:PRO:HB3     | 2:C:156:HIS:HD2     | 1.80                     | 0.46              |
| 1:F:155:TRP:NE1     | 2:E:177:LEU:HG      | 2.30                     | 0.46              |
| 1:D:213:VAL:HG13    | 1:D:231:LEU:HB3     | 1.98                     | 0.46              |
| 2:C:227:PRO:HD3     | 9:C:302:ATP:C6      | 2.49                     | 0.46              |
| 1:F:203:LYS:HD2     | 1:F:203:LYS:N       | 2.30                     | 0.46              |
| 2:I:193:ASP:HA      | 2:I:249:ASN:HB2     | 1.96                     | 0.46              |
| 2:A:86:HIS:HB2      | 2:E:11:VAL:HG22     | 1.97                     | 0.46              |
| 2:C:270:ARG:HE      | 2:C:270:ARG:HB2     | 1.60                     | 0.46              |
| 1:H:42:LYS:NZ       | 1:H:170:ASP:OD1     | 2.49                     | 0.46              |
| 1:B:38:ALA:HA       | 1:B:71:LYS:HB3      | 1.97                     | 0.46              |
| 1:F:76:THR:HG21     | 1:F:111:ALA:HA      | 1.98                     | 0.46              |
| 1:L:163:VAL:HG22    | 2:K:30:ALA:HB1      | 1.98                     | 0.45              |
| 2:C:193:ASP:HA      | 2:C:249:ASN:HB2     | 1.98                     | 0.45              |
| 1:L:71:LYS:HE3      | 1:L:136:LEU:O       | 2.15                     | 0.45              |
| 1:D:71:LYS:NZ       | 1:D:142:ASN:OD1     | 2.50                     | 0.45              |
| 1:L:131:LEU:N       | 1:L:131:LEU:HD23    | 2.31                     | 0.45              |
| 2:K:33:ARG:NH1      | 2:K:274:ARG:HH12    | 2.13                     | 0.45              |
| 2:K:274:ARG:HG3     | 2:K:274:ARG:NH2     | 2.29                     | 0.45              |
| 2:I:9:LYS:NZ        | 1:L:9:GLU:OE2       | 2.40                     | 0.45              |
| 1:L:118:LEU:HB3     | 1:L:123:ILE:HB      | 1.99                     | 0.45              |
| 2:K:178:ALA:HB1     | 2:K:242:ILE:HD11    | 1.99                     | 0.45              |
| 1:B:42:LYS:NZ       | 1:B:170:ASP:OD1     | 2.50                     | 0.45              |
| 1:L:228:PHE:HE2     | 12:K:401:HOH:O      | 1.99                     | 0.45              |
| 2:E:136:GLN:O       | 2:E:140:HIS:ND1     | 2.40                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:A:193:ASP:HA      | 2:A:249:ASN:HB2     | 1.99                     | 0.45              |
| 1:D:42:LYS:NZ       | 1:D:170:ASP:OD1     | 2.50                     | 0.45              |
| 1:F:165:PRO:O       | 1:F:168:ARG:NH1     | 2.45                     | 0.45              |
| 2:A:248:VAL:HG11    | 2:A:259:ALA:HB2     | 1.99                     | 0.44              |
| 2:K:130:HIS:N       | 5:K:303:8M0:O12     | 2.42                     | 0.44              |
| 1:B:138:LEU:HD21    | 1:F:138:LEU:HD13    | 1.98                     | 0.44              |
| 2:A:232:LEU:HD11    | 2:A:236:MET:HE3     | 1.99                     | 0.44              |
| 1:J:128:GLY:HA3     | 1:J:131:LEU:O       | 2.18                     | 0.44              |
| 2:A:139:ILE:HD13    | 2:C:140:HIS:HD2     | 1.82                     | 0.44              |
| 2:G:143:ALA:HB1     | 2:K:143:ALA:HB2     | 2.00                     | 0.44              |
| 2:K:193:ASP:HA      | 2:K:249:ASN:HB2     | 1.99                     | 0.44              |
| 1:D:130:GLY:HA3     | 1:D:180:PHE:CE2     | 2.52                     | 0.44              |
| 1:J:70:HIS:CD2      | 12:J:410:HOH:O      | 2.70                     | 0.44              |
| 1:L:149:MET:HE1     | 1:L:168:ARG:HG2     | 1.99                     | 0.43              |
| 1:D:133:ALA:O       | 1:D:137:SER:HB3     | 2.18                     | 0.43              |
| 2:E:215:SER:OG      | 2:E:218:ASP:HB2     | 2.18                     | 0.43              |
| 1:J:124:PRO:HG3     | 1:L:134:VAL:HG23    | 1.99                     | 0.43              |
| 1:L:4:SER:OG        | 1:L:7:GLU:HB3       | 2.17                     | 0.43              |
| 2:G:193:ASP:HA      | 2:G:249:ASN:HB2     | 2.00                     | 0.43              |
| 2:G:238:THR:O       | 2:G:240:ARG:NH1     | 2.49                     | 0.43              |
| 1:D:41:ILE:HG22     | 1:D:186:ILE:HB      | 2.01                     | 0.43              |
| 2:E:193:ASP:HA      | 2:E:249:ASN:HB2     | 1.99                     | 0.43              |
| 1:H:134:VAL:O       | 1:H:138:LEU:HD22    | 2.18                     | 0.43              |
| 2:I:143:ALA:HB2     | 2:K:143:ALA:HB1     | 2.01                     | 0.43              |
| 1:B:10:GLU:O        | 1:B:14[B]:GLN:HG2   | 2.19                     | 0.43              |
| 1:J:76:THR:HG21     | 1:J:111:ALA:HA      | 2.00                     | 0.43              |
| 2:I:207:GLN:H       | 2:I:207:GLN:HG2     | 1.61                     | 0.43              |
| 2:C:145[B]:ARG:HH12 | 2:G:145[B]:ARG:HH12 | 1.67                     | 0.42              |
| 2:C:132:THR:HG23    | 2:C:140:HIS:CE1     | 2.54                     | 0.42              |
| 2:G:248:VAL:HG11    | 2:G:259:ALA:HB2     | 2.01                     | 0.42              |
| 9:G:301:ATP:N3      | 9:G:301:ATP:H2'     | 2.34                     | 0.42              |
| 1:J:76:THR:HG22     | 1:J:114[B]:LEU:HD12 | 2.00                     | 0.42              |
| 9:I:301:ATP:N3      | 9:I:301:ATP:H2'     | 2.34                     | 0.42              |
| 2:A:209:ARG:HG2     | 2:A:209:ARG:HH21    | 1.83                     | 0.42              |
| 2:I:59:LEU:HB2      | 2:I:60:PRO:HD3      | 2.01                     | 0.42              |
| 2:G:209:ARG:HA      | 2:G:209:ARG:HD3     | 1.92                     | 0.42              |
| 2:K:136[B]:GLN:NE2  | 12:K:404:HOH:O      | 2.33                     | 0.42              |
| 1:B:244:GLN:NE2     | 12:B:409:HOH:O      | 2.52                     | 0.42              |
| 1:J:157:ARG:HD2     | 2:I:168:HIS:NE2     | 2.35                     | 0.42              |
| 1:J:176:LEU:HD12    | 1:J:176:LEU:HA      | 1.90                     | 0.42              |
| 1:B:134:VAL:HB      | 1:B:135:PRO:HD3     | 2.01                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:K:248:VAL:HG11   | 2:K:259:ALA:HB2     | 2.00                     | 0.42              |
| 1:H:163:VAL:HG22   | 2:G:30:ALA:HB1      | 2.01                     | 0.42              |
| 2:G:67:LYS:CE      | 12:G:406:HOH:O      | 2.67                     | 0.42              |
| 1:L:162:GLY:O      | 2:K:240:ARG:NH2     | 2.50                     | 0.42              |
| 1:F:129:ALA:C      | 1:F:131:LEU:N       | 2.78                     | 0.42              |
| 1:J:90:ALA:O       | 2:I:32:LYS:HE3      | 2.19                     | 0.42              |
| 1:D:155:TRP:NE1    | 2:C:177:LEU:HG      | 2.34                     | 0.42              |
| 2:I:232:LEU:HD11   | 2:I:236:MET:HE3     | 2.02                     | 0.42              |
| 1:F:129:ALA:O      | 1:F:131:LEU:CB      | 2.66                     | 0.41              |
| 9:E:301:ATP:N3     | 9:E:301:ATP:H2'     | 2.35                     | 0.41              |
| 1:L:155:TRP:NE1    | 2:K:177:LEU:HG      | 2.35                     | 0.41              |
| 1:H:165:PRO:O      | 1:H:168:ARG:NH1     | 2.43                     | 0.41              |
| 1:B:9:GLU:OE2      | 2:E:9:LYS:NZ        | 2.39                     | 0.41              |
| 1:B:76:THR:HG21    | 1:B:111:ALA:HA      | 2.02                     | 0.41              |
| 1:H:51:ARG:NH1     | 2:G:6:ASN:O         | 2.46                     | 0.41              |
| 2:G:67:LYS:HB3     | 2:G:67:LYS:HE3      | 1.82                     | 0.41              |
| 1:J:118:LEU:HB3    | 1:J:123:ILE:HB      | 2.02                     | 0.41              |
| 1:H:155:TRP:NE1    | 2:G:177:LEU:HG      | 2.36                     | 0.41              |
| 1:J:67:ARG:HD3     | 1:J:141:VAL:O       | 2.20                     | 0.41              |
| 1:F:176:LEU:HA     | 1:F:176:LEU:HD12    | 1.69                     | 0.41              |
| 2:E:59:LEU:HB2     | 2:E:60:PRO:HD3      | 2.02                     | 0.41              |
| 1:H:118:LEU:HB3    | 1:H:123:ILE:HB      | 2.02                     | 0.41              |
| 1:L:12:LEU:HD23    | 1:L:22:LEU:HD11     | 2.03                     | 0.41              |
| 1:B:130:GLY:HA3    | 1:B:180:PHE:CD2     | 2.56                     | 0.41              |
| 1:H:128:GLY:N      | 5:H:303:8M0:O18     | 2.53                     | 0.41              |
| 1:J:39:THR:HG23    | 1:J:184:GLN:HB3     | 2.01                     | 0.41              |
| 1:L:42:LYS:NZ      | 1:L:170:ASP:OD1     | 2.54                     | 0.41              |
| 2:E:145[B]:ARG:NH1 | 2:K:145[B]:ARG:HH12 | 2.17                     | 0.41              |
| 1:L:213:VAL:HG13   | 1:L:231:LEU:HB3     | 2.02                     | 0.41              |
| 1:D:130:GLY:HA3    | 1:D:180:PHE:CZ      | 2.55                     | 0.40              |
| 2:I:219:LEU:O      | 2:I:222:SER:HB3     | 2.20                     | 0.40              |
| 3:B:301:ADP:H8     | 2:A:19:THR:HG21     | 1.85                     | 0.40              |
| 1:L:4:SER:OG       | 1:L:7:GLU:HB2       | 2.21                     | 0.40              |
| 1:L:118:LEU:HD22   | 1:L:123:ILE:HD12    | 2.03                     | 0.40              |
| 1:D:76:THR:HG21    | 1:D:111:ALA:HA      | 2.03                     | 0.40              |
| 1:F:130:GLY:C      | 1:F:131:LEU:CG      | 2.90                     | 0.40              |
| 1:F:203:LYS:H      | 1:F:203:LYS:HD2     | 1.85                     | 0.40              |
| 2:A:63:GLU:O       | 2:A:67:LYS:HG3      | 2.22                     | 0.40              |
| 2:C:248:VAL:HG11   | 2:C:259:ALA:HB2     | 2.02                     | 0.40              |
| 1:H:131:LEU:HD21   | 1:L:125:VAL:H       | 1.87                     | 0.40              |
| 2:I:248:VAL:HG11   | 2:I:259:ALA:HB2     | 2.04                     | 0.40              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:F:40:VAL:HB  | 1:F:177:ALA:HB2 | 2.04                     | 0.40              |
| 1:F:203:LYS:CD | 1:F:203:LYS:N   | 2.84                     | 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 X-ray entries followed by that with respect to entries of similar resolution.

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   | B     | 271/269 (101%)   | 257 (95%)  | 12 (4%)  | 2 (1%)   | 18          | 7   |
| 1   | D     | 270/269 (100%)   | 256 (95%)  | 12 (4%)  | 2 (1%)   | 18          | 7   |
| 1   | F     | 271/269 (101%)   | 256 (94%)  | 13 (5%)  | 2 (1%)   | 18          | 7   |
| 1   | H     | 269/269 (100%)   | 258 (96%)  | 11 (4%)  | 0        | 100         | 100 |
| 1   | J     | 271/269 (101%)   | 259 (96%)  | 12 (4%)  | 0        | 100         | 100 |
| 1   | L     | 271/269 (101%)   | 261 (96%)  | 9 (3%)   | 1 (0%)   | 30          | 16  |
| 2   | A     | 272/275 (99%)    | 265 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 2   | C     | 271/275 (98%)    | 263 (97%)  | 8 (3%)   | 0        | 100         | 100 |
| 2   | E     | 272/275 (99%)    | 264 (97%)  | 8 (3%)   | 0        | 100         | 100 |
| 2   | G     | 273/275 (99%)    | 264 (97%)  | 9 (3%)   | 0        | 100         | 100 |
| 2   | I     | 272/275 (99%)    | 262 (96%)  | 10 (4%)  | 0        | 100         | 100 |
| 2   | K     | 275/275 (100%)   | 266 (97%)  | 8 (3%)   | 1 (0%)   | 30          | 16  |
| All | All   | 3258/3264 (100%) | 3131 (96%) | 119 (4%) | 8 (0%)   | 43          | 28  |

All (8) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 4   | SER  |
| 1   | F     | 130 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | K     | 274 | ARG  |
| 1   | D     | 128 | GLY  |
| 1   | F     | 132 | SER  |
| 1   | L     | 129 | ALA  |
| 1   | B     | 128 | GLY  |
| 1   | D     | 129 | ALA  |

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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   | B     | 210/205 (102%)   | 210 (100%)  | 0        | 100         | 100 |
| 1   | D     | 209/205 (102%)   | 209 (100%)  | 0        | 100         | 100 |
| 1   | F     | 209/205 (102%)   | 208 (100%)  | 1 (0%)   | 81          | 76  |
| 1   | H     | 208/205 (102%)   | 208 (100%)  | 0        | 100         | 100 |
| 1   | J     | 210/205 (102%)   | 210 (100%)  | 0        | 100         | 100 |
| 1   | L     | 210/205 (102%)   | 210 (100%)  | 0        | 100         | 100 |
| 2   | A     | 213/215 (99%)    | 212 (100%)  | 1 (0%)   | 81          | 76  |
| 2   | C     | 213/215 (99%)    | 213 (100%)  | 0        | 100         | 100 |
| 2   | E     | 214/215 (100%)   | 214 (100%)  | 0        | 100         | 100 |
| 2   | G     | 215/215 (100%)   | 215 (100%)  | 0        | 100         | 100 |
| 2   | I     | 214/215 (100%)   | 211 (99%)   | 3 (1%)   | 59          | 46  |
| 2   | K     | 217/215 (101%)   | 217 (100%)  | 0        | 100         | 100 |
| All | All   | 2542/2520 (101%) | 2537 (100%) | 5 (0%)   | 87          | 84  |

All (5) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 209 | ARG  |
| 1   | F     | 3   | ASN  |
| 2   | I     | 204 | ASP  |
| 2   | I     | 274 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | I     | 275 | PRO  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 3   | ASN  |
| 1   | B     | 46  | GLN  |
| 1   | B     | 184 | GLN  |
| 2   | A     | 201 | ASN  |
| 1   | D     | 3   | ASN  |
| 1   | D     | 101 | GLN  |
| 1   | D     | 184 | GLN  |
| 1   | D     | 235 | GLN  |
| 1   | D     | 262 | HIS  |
| 2   | C     | 18  | GLN  |
| 2   | C     | 157 | HIS  |
| 2   | C     | 201 | ASN  |
| 2   | C     | 207 | GLN  |
| 1   | F     | 14  | GLN  |
| 1   | F     | 101 | GLN  |
| 1   | F     | 238 | GLN  |
| 1   | H     | 21  | GLN  |
| 2   | G     | 18  | GLN  |
| 2   | G     | 201 | ASN  |
| 1   | J     | 70  | HIS  |
| 1   | J     | 184 | GLN  |
| 2   | I     | 207 | GLN  |
| 1   | L     | 21  | GLN  |
| 1   | L     | 46  | GLN  |
| 1   | L     | 69  | ASN  |
| 1   | L     | 101 | GLN  |
| 1   | L     | 184 | GLN  |
| 1   | L     | 262 | HIS  |
| 2   | K     | 6   | ASN  |
| 2   | K     | 18  | GLN  |
| 2   | K     | 241 | HIS  |

### 5.3.3 RNA ⓘ

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](#)

Of 54 ligands modelled in this entry, 12 are monoatomic - leaving 42 for Mogul analysis.

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$ |
| 7   | PO4  | J     | 305[B] | -    | 4,4,4        | 0.92 | 0           | 6,6,6       | 0.50 | 0           |
| 9   | ATP  | G     | 301    | 4    | 32,33,33     | 1.31 | 4 (12%)     | 48,52,52    | 1.99 | 12 (25%)    |
| 6   | MOO  | B     | 304[A] | -    | 2,4,4        | 1.96 | 1 (50%)     | -           |      |             |
| 5   | 8M0  | L     | 303    | -    | 34,48,48     | 2.47 | 9 (26%)     | -           |      |             |
| 3   | ADP  | L     | 301    | 4    | 28,29,29     | 1.35 | 5 (17%)     | 43,45,45    | 2.00 | 11 (25%)    |
| 7   | PO4  | L     | 305[B] | 4    | 4,4,4        | 0.99 | 0           | 6,6,6       | 0.48 | 0           |
| 5   | 8M0  | K     | 303    | -    | 16,46,48     | 3.15 | 5 (31%)     | -           |      |             |
| 5   | 8M0  | I     | 303    | -    | 16,46,48     | 3.11 | 5 (31%)     | -           |      |             |
| 9   | ATP  | E     | 301    | 4    | 32,33,33     | 1.36 | 5 (15%)     | 48,52,52    | 1.98 | 12 (25%)    |
| 6   | MOO  | J     | 304[A] | -    | 2,4,4        | 1.90 | 1 (50%)     | -           |      |             |
| 5   | 8M0  | F     | 303    | -    | 34,48,48     | 2.45 | 11 (32%)    | -           |      |             |
| 9   | ATP  | C     | 302    | 4    | 32,33,33     | 1.35 | 5 (15%)     | 48,52,52    | 1.96 | 12 (25%)    |
| 3   | ADP  | D     | 301    | 4    | 28,29,29     | 1.36 | 5 (17%)     | 43,45,45    | 2.02 | 11 (25%)    |
| 8   | LJB  | L     | 306    | -    | 15,44,44     | 9.66 | 4 (26%)     | -           |      |             |
| 9   | ATP  | I     | 301    | 4    | 32,33,33     | 1.40 | 6 (18%)     | 48,52,52    | 1.98 | 13 (27%)    |
| 9   | ATP  | K     | 301    | 4    | 32,33,33     | 1.38 | 5 (15%)     | 48,52,52    | 1.98 | 12 (25%)    |
| 5   | 8M0  | B     | 303    | -    | 34,48,48     | 2.52 | 11 (32%)    | -           |      |             |
| 7   | PO4  | B     | 305[B] | 4    | 4,4,4        | 0.97 | 0           | 6,6,6       | 0.49 | 0           |
| 5   | 8M0  | C     | 301    | -    | 34,48,48     | 2.51 | 11 (32%)    | -           |      |             |

| Mol | Type | Chain | Res    | Link | Bond lengths |        |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|--------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ   | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | ATP  | A     | 301    | 4    | 32,33,33     | 1.35   | 5 (15%)  | 48,52,52    | 2.00 | 12 (25%) |
| 5   | 8M0  | C     | 304    | -    | 16,46,48     | 3.11   | 5 (31%)  | -           |      |          |
| 6   | MOO  | H     | 304[A] | -    | 2,4,4        | 1.95   | 1 (50%)  | -           |      |          |
| 5   | 8M0  | A     | 303    | -    | 16,46,48     | 3.11   | 5 (31%)  | -           |      |          |
| 6   | MOO  | F     | 304[A] | -    | 2,4,4        | 1.98   | 1 (50%)  | -           |      |          |
| 10  | M10  | G     | 304    | -    | 3,15,18      | 103.51 | 3 (100%) | -           |      |          |
| 5   | 8M0  | J     | 302    | -    | 34,48,48     | 2.50   | 11 (32%) | -           |      |          |
| 10  | M10  | A     | 304    | -    | 4,15,18      | 6.56   | 4 (100%) | -           |      |          |
| 6   | MOO  | D     | 303[A] | -    | 2,4,4        | 1.95   | 1 (50%)  | -           |      |          |
| 11  | LHW  | K     | 304    | -    | 21,59,59     | 1.11   | 2 (9%)   | -           |      |          |
| 7   | PO4  | F     | 305[B] | 4    | 4,4,4        | 0.97   | 0        | 6,6,6       | 0.45 | 0        |
| 5   | 8M0  | H     | 303    | -    | 34,48,48     | 2.52   | 11 (32%) | -           |      |          |
| 7   | PO4  | H     | 305[B] | 4    | 4,4,4        | 0.97   | 0        | 6,6,6       | 0.46 | 0        |
| 3   | ADP  | F     | 301    | 4    | 28,29,29     | 1.36   | 5 (17%)  | 43,45,45    | 2.03 | 12 (27%) |
| 5   | 8M0  | G     | 303    | -    | 16,46,48     | 3.12   | 5 (31%)  | -           |      |          |
| 6   | MOO  | L     | 304[A] | -    | 2,4,4        | 1.91   | 1 (50%)  | -           |      |          |
| 3   | ADP  | H     | 301    | 4    | 28,29,29     | 1.35   | 5 (17%)  | 43,45,45    | 2.04 | 11 (25%) |
| 5   | 8M0  | E     | 303    | -    | 16,46,48     | 3.12   | 5 (31%)  | -           |      |          |
| 7   | PO4  | D     | 304[B] | 4    | 4,4,4        | 0.97   | 0        | 6,6,6       | 0.49 | 0        |
| 8   | LJB  | B     | 306    | -    | 15,44,44     | 10.47  | 4 (26%)  | -           |      |          |
| 3   | ADP  | B     | 301    | 4    | 28,29,29     | 1.38   | 6 (21%)  | 43,45,45    | 2.02 | 12 (27%) |
| 3   | ADP  | J     | 301    | 4    | 28,29,29     | 1.36   | 5 (17%)  | 43,45,45    | 2.02 | 11 (25%) |
| 11  | LHW  | C     | 305    | -    | 21,59,59     | 1.24   | 2 (9%)   | -           |      |          |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 9   | ATP  | A     | 301 | 4    | -       | 3/22/38/38 | 0/3/3/3 |
| 9   | ATP  | E     | 301 | 4    | -       | 2/22/38/38 | 0/3/3/3 |
| 9   | ATP  | G     | 301 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | ADP  | F     | 301 | 4    | -       | 5/16/32/32 | 0/3/3/3 |
| 9   | ATP  | C     | 302 | 4    | -       | 8/22/38/38 | 0/3/3/3 |
| 3   | ADP  | L     | 301 | 4    | -       | 5/16/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | ADP  | H     | 301 | 4    | -       | 6/16/32/32 | 0/3/3/3 |
| 3   | ADP  | D     | 301 | 4    | -       | 5/16/32/32 | 0/3/3/3 |
| 9   | ATP  | I     | 301 | 4    | -       | 2/22/38/38 | 0/3/3/3 |
| 10  | M10  | G     | 304 | -    | -       | -          | 0/4/3/3 |
| 9   | ATP  | K     | 301 | 4    | -       | 4/22/38/38 | 0/3/3/3 |
| 10  | M10  | A     | 304 | -    | -       | -          | 0/4/3/3 |
| 3   | ADP  | B     | 301 | 4    | -       | 5/16/32/32 | 0/3/3/3 |
| 3   | ADP  | J     | 301 | 4    | -       | 5/16/32/32 | 0/3/3/3 |

All (180) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 10  | G     | 304 | M10  | O11-MO3 | 179.20 | 4.06        | 1.68     |
| 8   | B     | 306 | LJB  | O14-MO8 | 28.81  | 2.22        | 1.80     |
| 8   | B     | 306 | LJB  | O24-MO8 | 28.25  | 2.24        | 1.80     |
| 8   | L     | 306 | LJB  | O14-MO8 | 27.82  | 2.20        | 1.80     |
| 8   | L     | 306 | LJB  | O24-MO8 | 24.72  | 2.18        | 1.80     |
| 10  | A     | 304 | M10  | O4-MO3  | 11.39  | 2.37        | 2.00     |
| 5   | C     | 304 | 8M0  | O23-MO7 | 8.02   | 1.88        | 1.71     |
| 5   | K     | 303 | 8M0  | O23-MO7 | 7.90   | 1.88        | 1.71     |
| 5   | B     | 303 | 8M0  | O23-MO7 | 7.90   | 1.88        | 1.71     |
| 5   | E     | 303 | 8M0  | O23-MO7 | 7.87   | 1.88        | 1.71     |
| 5   | F     | 303 | 8M0  | O23-MO7 | 7.87   | 1.88        | 1.71     |
| 5   | C     | 301 | 8M0  | O23-MO7 | 7.85   | 1.88        | 1.71     |
| 5   | H     | 303 | 8M0  | O23-MO7 | 7.84   | 1.88        | 1.71     |
| 5   | A     | 303 | 8M0  | O23-MO7 | 7.82   | 1.88        | 1.71     |
| 5   | G     | 303 | 8M0  | O23-MO7 | 7.80   | 1.88        | 1.71     |
| 5   | I     | 303 | 8M0  | O23-MO7 | 7.79   | 1.88        | 1.71     |
| 5   | J     | 302 | 8M0  | O23-MO7 | 7.79   | 1.88        | 1.71     |
| 5   | K     | 303 | 8M0  | O1-MO1  | 7.12   | 1.86        | 1.71     |
| 5   | C     | 301 | 8M0  | O1-MO1  | 7.11   | 1.86        | 1.71     |
| 5   | H     | 303 | 8M0  | O1-MO1  | 7.05   | 1.86        | 1.71     |
| 5   | F     | 303 | 8M0  | O1-MO1  | 7.04   | 1.86        | 1.71     |
| 5   | B     | 303 | 8M0  | O1-MO1  | 7.04   | 1.86        | 1.71     |
| 5   | J     | 302 | 8M0  | O1-MO1  | 7.02   | 1.86        | 1.71     |
| 5   | G     | 303 | 8M0  | O1-MO1  | 7.00   | 1.86        | 1.71     |
| 5   | L     | 303 | 8M0  | O23-MO7 | 6.96   | 1.86        | 1.71     |
| 5   | A     | 303 | 8M0  | O1-MO1  | 6.95   | 1.86        | 1.71     |
| 5   | I     | 303 | 8M0  | O1-MO1  | 6.92   | 1.86        | 1.71     |
| 5   | E     | 303 | 8M0  | O1-MO1  | 6.91   | 1.86        | 1.71     |
| 5   | C     | 304 | 8M0  | O1-MO1  | 6.90   | 1.86        | 1.71     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | L     | 303 | 8M0  | O1-MO1  | 6.81  | 1.86        | 1.71     |
| 5   | L     | 303 | 8M0  | O18-MO6 | 5.98  | 1.84        | 1.71     |
| 11  | C     | 305 | LHW  | O92-MOA | -4.66 | 1.86        | 2.26     |
| 3   | B     | 301 | ADP  | C5-C4   | 4.41  | 1.47        | 1.39     |
| 5   | H     | 303 | 8M0  | O18-MO6 | 4.40  | 1.80        | 1.71     |
| 3   | L     | 301 | ADP  | C5-C4   | 4.39  | 1.46        | 1.39     |
| 9   | I     | 301 | ATP  | C5-C4   | 4.36  | 1.46        | 1.39     |
| 9   | K     | 301 | ATP  | C5-C4   | 4.36  | 1.46        | 1.39     |
| 3   | H     | 301 | ADP  | C5-C4   | 4.36  | 1.46        | 1.39     |
| 5   | B     | 303 | 8M0  | O18-MO6 | 4.36  | 1.80        | 1.71     |
| 3   | F     | 301 | ADP  | C5-C4   | 4.36  | 1.46        | 1.39     |
| 9   | C     | 302 | ATP  | C5-C4   | 4.35  | 1.46        | 1.39     |
| 5   | G     | 303 | 8M0  | O18-MO6 | 4.35  | 1.80        | 1.71     |
| 5   | E     | 303 | 8M0  | O18-MO6 | 4.34  | 1.80        | 1.71     |
| 5   | J     | 302 | 8M0  | O18-MO6 | 4.34  | 1.80        | 1.71     |
| 3   | J     | 301 | ADP  | C5-C4   | 4.33  | 1.46        | 1.39     |
| 5   | C     | 301 | 8M0  | O18-MO6 | 4.33  | 1.80        | 1.71     |
| 5   | I     | 303 | 8M0  | O18-MO6 | 4.32  | 1.80        | 1.71     |
| 3   | D     | 301 | ADP  | C5-C4   | 4.31  | 1.46        | 1.39     |
| 9   | A     | 301 | ATP  | C5-C4   | 4.30  | 1.46        | 1.39     |
| 9   | E     | 301 | ATP  | C5-C4   | 4.30  | 1.46        | 1.39     |
| 5   | C     | 304 | 8M0  | O18-MO6 | 4.27  | 1.80        | 1.71     |
| 5   | K     | 303 | 8M0  | O18-MO6 | 4.26  | 1.80        | 1.71     |
| 5   | A     | 303 | 8M0  | O18-MO6 | 4.25  | 1.80        | 1.71     |
| 9   | G     | 301 | ATP  | C5-C4   | 4.24  | 1.46        | 1.39     |
| 10  | A     | 304 | M10  | O12-MO3 | 4.17  | 2.03        | 1.93     |
| 5   | L     | 303 | 8M0  | O27-MO3 | -4.15 | 1.74        | 2.34     |
| 11  | K     | 304 | LHW  | O92-MOA | -4.15 | 1.91        | 2.26     |
| 10  | A     | 304 | M10  | O9-MO3  | 3.99  | 2.03        | 1.93     |
| 5   | H     | 303 | 8M0  | O27-MO3 | -3.98 | 1.76        | 2.34     |
| 5   | C     | 301 | 8M0  | O27-MO3 | -3.98 | 1.76        | 2.34     |
| 5   | J     | 302 | 8M0  | O27-MO3 | -3.98 | 1.76        | 2.34     |
| 5   | B     | 303 | 8M0  | O27-MO3 | -3.97 | 1.77        | 2.34     |
| 5   | F     | 303 | 8M0  | O18-MO6 | 3.96  | 1.79        | 1.71     |
| 10  | G     | 304 | M10  | O3-MO3  | -3.96 | 1.72        | 2.34     |
| 10  | G     | 304 | M10  | O13-MO3 | -3.85 | 1.74        | 2.34     |
| 5   | H     | 303 | 8M0  | O20-MO6 | 3.49  | 2.22        | 1.89     |
| 5   | I     | 303 | 8M0  | O20-MO6 | 3.46  | 2.22        | 1.89     |
| 5   | L     | 303 | 8M0  | O20-MO6 | 3.46  | 2.22        | 1.89     |
| 5   | A     | 303 | 8M0  | O20-MO6 | 3.46  | 2.22        | 1.89     |
| 5   | F     | 303 | 8M0  | O20-MO6 | 3.45  | 2.22        | 1.89     |
| 5   | C     | 304 | 8M0  | O20-MO6 | 3.45  | 2.22        | 1.89     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | C     | 301 | 8M0  | O20-MO6 | 3.44  | 2.22        | 1.89     |
| 5   | K     | 303 | 8M0  | O20-MO6 | 3.43  | 2.22        | 1.89     |
| 5   | B     | 303 | 8M0  | O20-MO6 | 3.42  | 2.22        | 1.89     |
| 5   | G     | 303 | 8M0  | O20-MO6 | 3.39  | 2.21        | 1.89     |
| 5   | E     | 303 | 8M0  | O20-MO6 | 3.37  | 2.21        | 1.89     |
| 5   | J     | 302 | 8M0  | O20-MO6 | 3.35  | 2.21        | 1.89     |
| 5   | F     | 303 | 8M0  | O27-MO3 | -3.30 | 1.86        | 2.34     |
| 5   | J     | 302 | 8M0  | O7-MO2  | 3.09  | 2.18        | 1.89     |
| 5   | H     | 303 | 8M0  | O3-MO3  | 3.03  | 2.03        | 1.93     |
| 10  | A     | 304 | M10  | O11-MO3 | 3.00  | 1.74        | 1.67     |
| 5   | H     | 303 | 8M0  | O7-MO2  | 2.97  | 2.17        | 1.89     |
| 5   | F     | 303 | 8M0  | O7-MO2  | 2.95  | 2.17        | 1.89     |
| 5   | B     | 303 | 8M0  | O7-MO2  | 2.95  | 2.17        | 1.89     |
| 5   | J     | 302 | 8M0  | O26-MO6 | -2.93 | 1.95        | 2.24     |
| 5   | C     | 301 | 8M0  | O7-MO2  | 2.90  | 2.17        | 1.89     |
| 8   | B     | 306 | LJB  | O53-MO5 | -2.89 | 2.01        | 2.26     |
| 5   | K     | 303 | 8M0  | O7-MO2  | 2.84  | 2.16        | 1.89     |
| 5   | L     | 303 | 8M0  | O7-MO2  | 2.84  | 2.16        | 1.89     |
| 5   | C     | 301 | 8M0  | O3-MO3  | 2.82  | 2.03        | 1.93     |
| 5   | L     | 303 | 8M0  | O26-MO6 | -2.80 | 1.96        | 2.24     |
| 5   | B     | 303 | 8M0  | O26-MO6 | -2.79 | 1.96        | 2.24     |
| 8   | L     | 306 | LJB  | O53-MO5 | -2.79 | 2.02        | 2.26     |
| 5   | E     | 303 | 8M0  | O7-MO2  | 2.78  | 2.16        | 1.89     |
| 5   | A     | 303 | 8M0  | O7-MO2  | 2.78  | 2.15        | 1.89     |
| 5   | I     | 303 | 8M0  | O7-MO2  | 2.77  | 2.15        | 1.89     |
| 5   | C     | 301 | 8M0  | O26-MO6 | -2.77 | 1.97        | 2.24     |
| 5   | B     | 303 | 8M0  | O3-MO3  | 2.77  | 2.02        | 1.93     |
| 5   | G     | 303 | 8M0  | O7-MO2  | 2.76  | 2.15        | 1.89     |
| 5   | H     | 303 | 8M0  | O26-MO6 | -2.70 | 1.97        | 2.24     |
| 11  | C     | 305 | LHW  | O92-MO8 | -2.66 | 2.03        | 2.26     |
| 5   | B     | 303 | 8M0  | O15-MO5 | -2.65 | 1.96        | 2.34     |
| 5   | C     | 301 | 8M0  | O15-MO5 | -2.63 | 1.96        | 2.34     |
| 9   | I     | 301 | ATP  | C5-C6   | 2.61  | 1.48        | 1.41     |
| 5   | H     | 303 | 8M0  | O15-MO5 | -2.61 | 1.96        | 2.34     |
| 5   | F     | 303 | 8M0  | O15-MO5 | -2.61 | 1.96        | 2.34     |
| 5   | J     | 302 | 8M0  | O15-MO5 | -2.60 | 1.96        | 2.34     |
| 5   | L     | 303 | 8M0  | O15-MO5 | -2.60 | 1.96        | 2.34     |
| 8   | L     | 306 | LJB  | O53-MO6 | -2.59 | 2.04        | 2.26     |
| 5   | F     | 303 | 8M0  | O26-MO6 | -2.58 | 1.99        | 2.24     |
| 3   | H     | 301 | ADP  | C5-C6   | 2.55  | 1.48        | 1.41     |
| 9   | K     | 301 | ATP  | C5-C6   | 2.55  | 1.48        | 1.41     |
| 9   | C     | 302 | ATP  | C5-C6   | 2.54  | 1.48        | 1.41     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 3   | F     | 301    | ADP  | C5-C6   | 2.54  | 1.48        | 1.41     |
| 9   | G     | 301    | ATP  | C5-N7   | -2.54 | 1.34        | 1.39     |
| 3   | D     | 301    | ADP  | C5-C6   | 2.53  | 1.48        | 1.41     |
| 9   | A     | 301    | ATP  | C5-N7   | -2.53 | 1.34        | 1.39     |
| 3   | J     | 301    | ADP  | C5-C6   | 2.52  | 1.48        | 1.41     |
| 3   | L     | 301    | ADP  | C5-C6   | 2.50  | 1.47        | 1.41     |
| 9   | E     | 301    | ATP  | C5-N7   | -2.49 | 1.34        | 1.39     |
| 3   | B     | 301    | ADP  | C5-C6   | 2.48  | 1.47        | 1.41     |
| 9   | K     | 301    | ATP  | PB-O3B  | 2.48  | 1.62        | 1.59     |
| 9   | E     | 301    | ATP  | C5-C6   | 2.48  | 1.47        | 1.41     |
| 9   | G     | 301    | ATP  | C5-C6   | 2.47  | 1.47        | 1.41     |
| 9   | I     | 301    | ATP  | C5-N7   | -2.47 | 1.34        | 1.39     |
| 3   | D     | 301    | ADP  | C5-N7   | -2.46 | 1.34        | 1.39     |
| 5   | F     | 303    | 8M0  | O3-MO3  | 2.46  | 2.01        | 1.93     |
| 8   | B     | 306    | LJB  | O53-MO6 | -2.45 | 2.05        | 2.26     |
| 5   | C     | 304    | 8M0  | O7-MO2  | 2.44  | 2.12        | 1.89     |
| 9   | A     | 301    | ATP  | C5-C6   | 2.44  | 1.47        | 1.41     |
| 6   | F     | 304[A] | MOO  | O1-MO   | -2.43 | 1.70        | 1.75     |
| 5   | J     | 302    | 8M0  | O3-MO3  | 2.42  | 2.01        | 1.93     |
| 9   | K     | 301    | ATP  | C5-N7   | -2.40 | 1.34        | 1.39     |
| 3   | H     | 301    | ADP  | C5-N7   | -2.39 | 1.34        | 1.39     |
| 3   | J     | 301    | ADP  | C5-N7   | -2.38 | 1.34        | 1.39     |
| 6   | D     | 303[A] | MOO  | O1-MO   | -2.38 | 1.70        | 1.75     |
| 6   | H     | 304[A] | MOO  | O1-MO   | -2.37 | 1.70        | 1.75     |
| 3   | F     | 301    | ADP  | C5-N7   | -2.36 | 1.34        | 1.39     |
| 6   | B     | 304[A] | MOO  | O1-MO   | -2.35 | 1.70        | 1.75     |
| 5   | L     | 303    | 8M0  | O25-MO2 | -2.35 | 2.01        | 2.24     |
| 9   | I     | 301    | ATP  | PB-O3B  | 2.34  | 1.62        | 1.59     |
| 6   | L     | 304[A] | MOO  | O1-MO   | -2.33 | 1.70        | 1.75     |
| 9   | C     | 302    | ATP  | C5-N7   | -2.33 | 1.34        | 1.39     |
| 3   | L     | 301    | ADP  | C5-N7   | -2.33 | 1.34        | 1.39     |
| 6   | J     | 304[A] | MOO  | O1-MO   | -2.32 | 1.70        | 1.75     |
| 9   | A     | 301    | ATP  | PB-O3B  | 2.32  | 1.62        | 1.59     |
| 11  | K     | 304    | LHW  | O92-MO8 | -2.27 | 2.07        | 2.26     |
| 3   | B     | 301    | ADP  | C4-N9   | -2.26 | 1.33        | 1.37     |
| 3   | B     | 301    | ADP  | C5-N7   | -2.24 | 1.35        | 1.39     |
| 3   | L     | 301    | ADP  | C4-N9   | -2.22 | 1.33        | 1.37     |
| 5   | J     | 302    | 8M0  | O25-MO2 | -2.21 | 2.02        | 2.24     |
| 3   | F     | 301    | ADP  | C8-N7   | 2.20  | 1.35        | 1.31     |
| 9   | I     | 301    | ATP  | C8-N7   | 2.18  | 1.35        | 1.31     |
| 9   | C     | 302    | ATP  | PB-O3B  | 2.18  | 1.61        | 1.59     |
| 3   | H     | 301    | ADP  | C8-N7   | 2.17  | 1.35        | 1.31     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | B     | 303 | 8M0  | O25-MO2 | -2.16 | 2.03        | 2.24     |
| 3   | F     | 301 | ADP  | C4-N9   | -2.15 | 1.33        | 1.37     |
| 9   | K     | 301 | ATP  | C8-N7   | 2.15  | 1.35        | 1.31     |
| 9   | E     | 301 | ATP  | PB-O3B  | 2.14  | 1.61        | 1.59     |
| 9   | E     | 301 | ATP  | C8-N7   | 2.12  | 1.35        | 1.31     |
| 3   | J     | 301 | ADP  | C4-N9   | -2.12 | 1.33        | 1.37     |
| 9   | G     | 301 | ATP  | C8-N7   | 2.11  | 1.35        | 1.31     |
| 3   | J     | 301 | ADP  | C8-N7   | 2.11  | 1.35        | 1.31     |
| 3   | D     | 301 | ADP  | C4-N9   | -2.10 | 1.33        | 1.37     |
| 3   | B     | 301 | ADP  | C8-N7   | 2.09  | 1.35        | 1.31     |
| 3   | L     | 301 | ADP  | C8-N7   | 2.08  | 1.35        | 1.31     |
| 5   | H     | 303 | 8M0  | O25-MO2 | -2.08 | 2.03        | 2.24     |
| 3   | H     | 301 | ADP  | C4-N9   | -2.08 | 1.33        | 1.37     |
| 3   | B     | 301 | ADP  | PA-O3A  | 2.07  | 1.61        | 1.59     |
| 3   | D     | 301 | ADP  | C8-N7   | 2.07  | 1.35        | 1.31     |
| 5   | C     | 301 | 8M0  | O25-MO2 | -2.07 | 2.04        | 2.24     |
| 5   | F     | 303 | 8M0  | O25-MO2 | -2.05 | 2.04        | 2.24     |
| 9   | C     | 302 | ATP  | C8-N7   | 2.05  | 1.35        | 1.31     |
| 9   | A     | 301 | ATP  | C4-N9   | -2.04 | 1.33        | 1.37     |
| 9   | I     | 301 | ATP  | PB-O3A  | 2.01  | 1.61        | 1.59     |
| 5   | B     | 303 | 8M0  | O9-MO3  | 2.01  | 1.90        | 1.72     |
| 5   | J     | 302 | 8M0  | O9-MO3  | 2.01  | 1.90        | 1.72     |
| 5   | F     | 303 | 8M0  | O9-MO3  | 2.00  | 1.90        | 1.72     |
| 5   | C     | 301 | 8M0  | O9-MO3  | 2.00  | 1.90        | 1.72     |
| 5   | H     | 303 | 8M0  | O9-MO3  | 2.00  | 1.90        | 1.72     |

All (141) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 9   | I     | 301 | ATP  | C5-C4-N3 | -6.16 | 118.23      | 126.72   |
| 9   | E     | 301 | ATP  | C5-C4-N3 | -6.13 | 118.28      | 126.72   |
| 9   | K     | 301 | ATP  | C5-C4-N3 | -6.06 | 118.38      | 126.72   |
| 3   | D     | 301 | ADP  | C5-C4-N3 | -6.05 | 118.39      | 126.72   |
| 9   | G     | 301 | ATP  | C5-C4-N3 | -6.04 | 118.39      | 126.72   |
| 3   | J     | 301 | ADP  | C5-C4-N3 | -6.04 | 118.40      | 126.72   |
| 3   | H     | 301 | ADP  | C5-C4-N3 | -6.01 | 118.45      | 126.72   |
| 9   | A     | 301 | ATP  | C5-C4-N3 | -5.97 | 118.50      | 126.72   |
| 3   | F     | 301 | ADP  | C5-C4-N3 | -5.87 | 118.64      | 126.72   |
| 3   | L     | 301 | ADP  | C5-C4-N3 | -5.81 | 118.72      | 126.72   |
| 9   | C     | 302 | ATP  | C5-C4-N3 | -5.81 | 118.72      | 126.72   |
| 3   | B     | 301 | ADP  | C5-C4-N3 | -5.77 | 118.77      | 126.72   |
| 3   | D     | 301 | ADP  | N3-C4-N9 | 5.15  | 135.92      | 127.17   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | J     | 301 | ADP  | N3-C4-N9    | 5.11  | 135.85      | 127.17   |
| 9   | K     | 301 | ATP  | N3-C4-N9    | 5.10  | 135.85      | 127.17   |
| 9   | A     | 301 | ATP  | N3-C4-N9    | 5.10  | 135.84      | 127.17   |
| 9   | E     | 301 | ATP  | N3-C4-N9    | 5.09  | 135.82      | 127.17   |
| 3   | H     | 301 | ADP  | N3-C4-N9    | 5.09  | 135.82      | 127.17   |
| 9   | I     | 301 | ATP  | N3-C4-N9    | 5.05  | 135.75      | 127.17   |
| 3   | L     | 301 | ADP  | N3-C4-N9    | 5.04  | 135.74      | 127.17   |
| 9   | G     | 301 | ATP  | N3-C4-N9    | 5.04  | 135.73      | 127.17   |
| 3   | F     | 301 | ADP  | N3-C4-N9    | 5.02  | 135.71      | 127.17   |
| 3   | B     | 301 | ADP  | N3-C4-N9    | 5.01  | 135.69      | 127.17   |
| 9   | C     | 302 | ATP  | N3-C4-N9    | 4.95  | 135.59      | 127.17   |
| 9   | I     | 301 | ATP  | C2-N3-C4    | 4.20  | 122.10      | 111.83   |
| 9   | E     | 301 | ATP  | C2-N3-C4    | 4.15  | 121.97      | 111.83   |
| 9   | E     | 301 | ATP  | N3-C2-N1    | -4.15 | 122.30      | 128.58   |
| 9   | I     | 301 | ATP  | N3-C2-N1    | -4.12 | 122.34      | 128.58   |
| 9   | G     | 301 | ATP  | N3-C2-N1    | -4.11 | 122.36      | 128.58   |
| 9   | G     | 301 | ATP  | C2-N3-C4    | 4.11  | 121.87      | 111.83   |
| 9   | K     | 301 | ATP  | C2-N3-C4    | 4.10  | 121.85      | 111.83   |
| 3   | J     | 301 | ADP  | C2-N3-C4    | 4.10  | 121.83      | 111.83   |
| 3   | H     | 301 | ADP  | C2-N3-C4    | 4.08  | 121.79      | 111.83   |
| 3   | D     | 301 | ADP  | C2-N3-C4    | 4.07  | 121.76      | 111.83   |
| 3   | F     | 301 | ADP  | N3-C2-N1    | -4.02 | 122.50      | 128.58   |
| 9   | K     | 301 | ATP  | N3-C2-N1    | -4.01 | 122.50      | 128.58   |
| 3   | J     | 301 | ADP  | N3-C2-N1    | -4.01 | 122.51      | 128.58   |
| 3   | F     | 301 | ADP  | C2-N3-C4    | 4.00  | 121.60      | 111.83   |
| 9   | C     | 302 | ATP  | C2-N3-C4    | 4.00  | 121.59      | 111.83   |
| 9   | A     | 301 | ATP  | C2-N3-C4    | 3.98  | 121.55      | 111.83   |
| 3   | H     | 301 | ADP  | N3-C2-N1    | -3.98 | 122.56      | 128.58   |
| 9   | C     | 302 | ATP  | N3-C2-N1    | -3.97 | 122.57      | 128.58   |
| 3   | L     | 301 | ADP  | C2-N3-C4    | 3.95  | 121.49      | 111.83   |
| 3   | D     | 301 | ADP  | N3-C2-N1    | -3.95 | 122.61      | 128.58   |
| 3   | B     | 301 | ADP  | N3-C2-N1    | -3.94 | 122.62      | 128.58   |
| 3   | B     | 301 | ADP  | C2-N3-C4    | 3.94  | 121.44      | 111.83   |
| 3   | L     | 301 | ADP  | N3-C2-N1    | -3.93 | 122.63      | 128.58   |
| 9   | A     | 301 | ATP  | N3-C2-N1    | -3.88 | 122.70      | 128.58   |
| 3   | B     | 301 | ADP  | C4-N9-C8    | 3.66  | 109.59      | 105.74   |
| 3   | L     | 301 | ADP  | C4-N9-C8    | 3.57  | 109.49      | 105.74   |
| 3   | F     | 301 | ADP  | C4-N9-C8    | 3.55  | 109.46      | 105.74   |
| 9   | A     | 301 | ATP  | C3'-C2'-C1' | 3.46  | 108.01      | 101.46   |
| 3   | H     | 301 | ADP  | C4-N9-C8    | 3.43  | 109.34      | 105.74   |
| 9   | A     | 301 | ATP  | C4-N9-C8    | 3.41  | 109.31      | 105.74   |
| 9   | C     | 302 | ATP  | C3'-C2'-C1' | 3.40  | 107.89      | 101.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 9   | G     | 301 | ATP  | C3'-C2'-C1' | 3.40  | 107.89      | 101.46   |
| 3   | D     | 301 | ADP  | C4-N9-C8    | 3.39  | 109.30      | 105.74   |
| 9   | I     | 301 | ATP  | C4-C5-N7    | -3.38 | 106.72      | 110.58   |
| 3   | J     | 301 | ADP  | C4-N9-C8    | 3.36  | 109.27      | 105.74   |
| 9   | C     | 302 | ATP  | C4-N9-C8    | 3.35  | 109.26      | 105.74   |
| 9   | K     | 301 | ATP  | C3'-C2'-C1' | 3.35  | 107.80      | 101.46   |
| 9   | K     | 301 | ATP  | C4-N9-C8    | 3.35  | 109.25      | 105.74   |
| 9   | G     | 301 | ATP  | C4-C5-N7    | -3.33 | 106.77      | 110.58   |
| 9   | I     | 301 | ATP  | C3'-C2'-C1' | 3.33  | 107.76      | 101.46   |
| 9   | E     | 301 | ATP  | C3'-C2'-C1' | 3.28  | 107.67      | 101.46   |
| 9   | E     | 301 | ATP  | C4-C5-N7    | -3.28 | 106.83      | 110.58   |
| 9   | K     | 301 | ATP  | C4-C5-N7    | -3.26 | 106.86      | 110.58   |
| 9   | A     | 301 | ATP  | C4-C5-N7    | -3.25 | 106.86      | 110.58   |
| 9   | C     | 302 | ATP  | C4-C5-N7    | -3.18 | 106.95      | 110.58   |
| 9   | G     | 301 | ATP  | C4-N9-C8    | 3.18  | 109.07      | 105.74   |
| 9   | E     | 301 | ATP  | C4-N9-C8    | 3.16  | 109.06      | 105.74   |
| 3   | H     | 301 | ADP  | C4-C5-N7    | -3.14 | 106.99      | 110.58   |
| 3   | D     | 301 | ADP  | C4-C5-N7    | -3.13 | 107.00      | 110.58   |
| 3   | J     | 301 | ADP  | C4-C5-N7    | -3.11 | 107.03      | 110.58   |
| 9   | A     | 301 | ATP  | O4'-C1'-N9  | 3.10  | 114.04      | 108.09   |
| 3   | F     | 301 | ADP  | C4-C5-N7    | -3.06 | 107.08      | 110.58   |
| 3   | B     | 301 | ADP  | C4-C5-N7    | -3.02 | 107.12      | 110.58   |
| 9   | I     | 301 | ATP  | C4-N9-C8    | 3.02  | 108.91      | 105.74   |
| 3   | B     | 301 | ADP  | C3'-C2'-C1' | 3.00  | 107.14      | 101.46   |
| 3   | L     | 301 | ADP  | C4-C5-N7    | -2.98 | 107.17      | 110.58   |
| 9   | G     | 301 | ATP  | O4'-C1'-N9  | 2.98  | 113.81      | 108.09   |
| 3   | F     | 301 | ADP  | C3'-C2'-C1' | 2.89  | 106.93      | 101.46   |
| 9   | G     | 301 | ATP  | C5-N7-C8    | 2.84  | 107.92      | 103.45   |
| 9   | C     | 302 | ATP  | O4'-C1'-N9  | 2.82  | 113.51      | 108.09   |
| 3   | J     | 301 | ADP  | C3'-C2'-C1' | 2.82  | 106.79      | 101.46   |
| 3   | L     | 301 | ADP  | C3'-C2'-C1' | 2.81  | 106.78      | 101.46   |
| 9   | I     | 301 | ATP  | C5-N7-C8    | 2.78  | 107.82      | 103.45   |
| 9   | A     | 301 | ATP  | C5-N7-C8    | 2.75  | 107.77      | 103.45   |
| 9   | E     | 301 | ATP  | C5-N7-C8    | 2.74  | 107.76      | 103.45   |
| 9   | K     | 301 | ATP  | O4'-C1'-N9  | 2.74  | 113.35      | 108.09   |
| 9   | K     | 301 | ATP  | C5-N7-C8    | 2.72  | 107.73      | 103.45   |
| 9   | E     | 301 | ATP  | O4'-C1'-N9  | 2.72  | 113.31      | 108.09   |
| 3   | D     | 301 | ADP  | C3'-C2'-C1' | 2.67  | 106.51      | 101.46   |
| 9   | C     | 302 | ATP  | C5-N7-C8    | 2.65  | 107.61      | 103.45   |
| 3   | H     | 301 | ADP  | C5-N7-C8    | 2.65  | 107.61      | 103.45   |
| 3   | H     | 301 | ADP  | C3'-C2'-C1' | 2.64  | 106.46      | 101.46   |
| 3   | D     | 301 | ADP  | C5-N7-C8    | 2.62  | 107.57      | 103.45   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 9   | I     | 301 | ATP  | O4'-C1'-N9 | 2.59  | 113.06      | 108.09   |
| 3   | J     | 301 | ADP  | C5-N7-C8   | 2.58  | 107.51      | 103.45   |
| 3   | F     | 301 | ADP  | C5-N7-C8   | 2.57  | 107.49      | 103.45   |
| 3   | F     | 301 | ADP  | N9-C8-N7   | -2.56 | 110.31      | 113.94   |
| 3   | H     | 301 | ADP  | N9-C8-N7   | -2.54 | 110.34      | 113.94   |
| 9   | G     | 301 | ATP  | N9-C8-N7   | -2.52 | 110.36      | 113.94   |
| 9   | A     | 301 | ATP  | N9-C8-N7   | -2.51 | 110.37      | 113.94   |
| 9   | K     | 301 | ATP  | N9-C8-N7   | -2.50 | 110.38      | 113.94   |
| 3   | L     | 301 | ADP  | C5-N7-C8   | 2.49  | 107.36      | 103.45   |
| 3   | B     | 301 | ADP  | N9-C8-N7   | -2.48 | 110.41      | 113.94   |
| 3   | B     | 301 | ADP  | C5-N7-C8   | 2.48  | 107.35      | 103.45   |
| 3   | L     | 301 | ADP  | N9-C8-N7   | -2.47 | 110.44      | 113.94   |
| 3   | D     | 301 | ADP  | N9-C8-N7   | -2.46 | 110.44      | 113.94   |
| 9   | E     | 301 | ATP  | N9-C8-N7   | -2.46 | 110.44      | 113.94   |
| 3   | J     | 301 | ADP  | N9-C8-N7   | -2.46 | 110.44      | 113.94   |
| 3   | H     | 301 | ADP  | C1'-N9-C8  | -2.45 | 121.66      | 127.09   |
| 9   | C     | 302 | ATP  | N9-C8-N7   | -2.42 | 110.50      | 113.94   |
| 9   | A     | 301 | ATP  | C1'-N9-C8  | -2.42 | 121.73      | 127.09   |
| 3   | D     | 301 | ADP  | C1'-N9-C8  | -2.41 | 121.74      | 127.09   |
| 9   | I     | 301 | ATP  | N9-C8-N7   | -2.40 | 110.53      | 113.94   |
| 3   | J     | 301 | ADP  | C1'-N9-C8  | -2.38 | 121.81      | 127.09   |
| 3   | L     | 301 | ADP  | C1'-N9-C8  | -2.35 | 121.88      | 127.09   |
| 9   | K     | 301 | ATP  | C1'-N9-C8  | -2.32 | 121.95      | 127.09   |
| 3   | F     | 301 | ADP  | C1'-N9-C8  | -2.29 | 122.00      | 127.09   |
| 9   | E     | 301 | ATP  | C1'-N9-C8  | -2.29 | 122.01      | 127.09   |
| 3   | B     | 301 | ADP  | C1'-N9-C8  | -2.28 | 122.03      | 127.09   |
| 3   | F     | 301 | ADP  | C2-N1-C6   | 2.27  | 122.45      | 118.73   |
| 9   | C     | 302 | ATP  | C1'-N9-C8  | -2.26 | 122.07      | 127.09   |
| 9   | G     | 301 | ATP  | C1'-N9-C8  | -2.24 | 122.13      | 127.09   |
| 3   | L     | 301 | ADP  | C2-N1-C6   | 2.22  | 122.38      | 118.73   |
| 9   | E     | 301 | ATP  | C2-N1-C6   | 2.20  | 122.35      | 118.73   |
| 3   | B     | 301 | ADP  | C2-N1-C6   | 2.20  | 122.34      | 118.73   |
| 3   | B     | 301 | ADP  | C2'-C1'-N9 | 2.19  | 118.75      | 113.30   |
| 9   | I     | 301 | ATP  | C1'-N9-C8  | -2.19 | 122.24      | 127.09   |
| 9   | G     | 301 | ATP  | C2-N1-C6   | 2.17  | 122.30      | 118.73   |
| 9   | I     | 301 | ATP  | C2-N1-C6   | 2.17  | 122.30      | 118.73   |
| 3   | J     | 301 | ADP  | C2-N1-C6   | 2.14  | 122.25      | 118.73   |
| 9   | C     | 302 | ATP  | C2-N1-C6   | 2.12  | 122.21      | 118.73   |
| 3   | F     | 301 | ADP  | C2'-C1'-N9 | 2.11  | 118.55      | 113.30   |
| 3   | D     | 301 | ADP  | C2-N1-C6   | 2.11  | 122.19      | 118.73   |
| 3   | H     | 301 | ADP  | C2-N1-C6   | 2.10  | 122.18      | 118.73   |
| 9   | K     | 301 | ATP  | C2-N1-C6   | 2.10  | 122.17      | 118.73   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 9   | A     | 301 | ATP  | C2-N1-C6 | 2.04 | 122.09      | 118.73   |
| 9   | I     | 301 | ATP  | C6-C5-N7 | 2.02 | 135.99      | 132.09   |

There are no chirality outliers.

All (56) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 3   | B     | 301 | ADP  | C2'-C1'-N9-C4  |
| 3   | D     | 301 | ADP  | C2'-C1'-N9-C4  |
| 3   | F     | 301 | ADP  | C2'-C1'-N9-C4  |
| 3   | H     | 301 | ADP  | C2'-C1'-N9-C4  |
| 3   | J     | 301 | ADP  | C2'-C1'-N9-C4  |
| 3   | L     | 301 | ADP  | C2'-C1'-N9-C4  |
| 9   | E     | 301 | ATP  | C2'-C1'-N9-C4  |
| 9   | G     | 301 | ATP  | C2'-C1'-N9-C4  |
| 9   | I     | 301 | ATP  | C2'-C1'-N9-C4  |
| 9   | K     | 301 | ATP  | C2'-C1'-N9-C4  |
| 3   | D     | 301 | ADP  | C4'-C5'-O5'-PA |
| 3   | F     | 301 | ADP  | C2'-C1'-N9-C8  |
| 3   | B     | 301 | ADP  | PB-O3A-PA-O2A  |
| 3   | F     | 301 | ADP  | PB-O3A-PA-O2A  |
| 3   | J     | 301 | ADP  | PB-O3A-PA-O1A  |
| 3   | L     | 301 | ADP  | PB-O3A-PA-O2A  |
| 3   | B     | 301 | ADP  | C4'-C5'-O5'-PA |
| 3   | J     | 301 | ADP  | C4'-C5'-O5'-PA |
| 3   | B     | 301 | ADP  | C2'-C1'-N9-C8  |
| 3   | D     | 301 | ADP  | C2'-C1'-N9-C8  |
| 3   | H     | 301 | ADP  | C2'-C1'-N9-C8  |
| 3   | J     | 301 | ADP  | C2'-C1'-N9-C8  |
| 3   | L     | 301 | ADP  | C2'-C1'-N9-C8  |
| 3   | H     | 301 | ADP  | C5'-O5'-PA-O1A |
| 3   | F     | 301 | ADP  | C4'-C5'-O5'-PA |
| 3   | H     | 301 | ADP  | C4'-C5'-O5'-PA |
| 3   | L     | 301 | ADP  | C4'-C5'-O5'-PA |
| 9   | G     | 301 | ATP  | C2'-C1'-N9-C8  |
| 9   | I     | 301 | ATP  | C2'-C1'-N9-C8  |
| 9   | K     | 301 | ATP  | C2'-C1'-N9-C8  |
| 3   | H     | 301 | ADP  | PB-O3A-PA-O2A  |
| 9   | A     | 301 | ATP  | C2'-C1'-N9-C4  |
| 9   | C     | 302 | ATP  | C2'-C1'-N9-C4  |
| 9   | A     | 301 | ATP  | C2'-C1'-N9-C8  |
| 9   | C     | 302 | ATP  | C2'-C1'-N9-C8  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 9   | E     | 301 | ATP  | C2'-C1'-N9-C8   |
| 3   | F     | 301 | ADP  | PB-O3A-PA-O1A   |
| 3   | D     | 301 | ADP  | PA-O3A-PB-O2B   |
| 9   | A     | 301 | ATP  | O4'-C1'-N9-C8   |
| 9   | C     | 302 | ATP  | O4'-C1'-N9-C8   |
| 9   | C     | 302 | ATP  | C3'-C4'-C5'-O5' |
| 3   | D     | 301 | ADP  | PB-O3A-PA-O2A   |
| 3   | H     | 301 | ADP  | PB-O3A-PA-O1A   |
| 3   | J     | 301 | ADP  | PB-O3A-PA-O2A   |
| 9   | C     | 302 | ATP  | PA-O3A-PB-O2B   |
| 9   | C     | 302 | ATP  | PB-O3A-PA-O1A   |
| 9   | G     | 301 | ATP  | PA-O3A-PB-O2B   |
| 9   | G     | 301 | ATP  | PB-O3A-PA-O1A   |
| 9   | K     | 301 | ATP  | O4'-C1'-N9-C8   |
| 9   | G     | 301 | ATP  | O4'-C1'-N9-C8   |
| 3   | B     | 301 | ADP  | PB-O3A-PA-O1A   |
| 3   | L     | 301 | ADP  | PB-O3A-PA-O1A   |
| 9   | C     | 302 | ATP  | PG-O3B-PB-O2B   |
| 9   | C     | 302 | ATP  | PB-O3A-PA-O2A   |
| 9   | G     | 301 | ATP  | PG-O3B-PB-O2B   |
| 9   | K     | 301 | ATP  | PA-O3A-PB-O2B   |

There are no ring outliers.

27 monomers are involved in 69 short contacts:

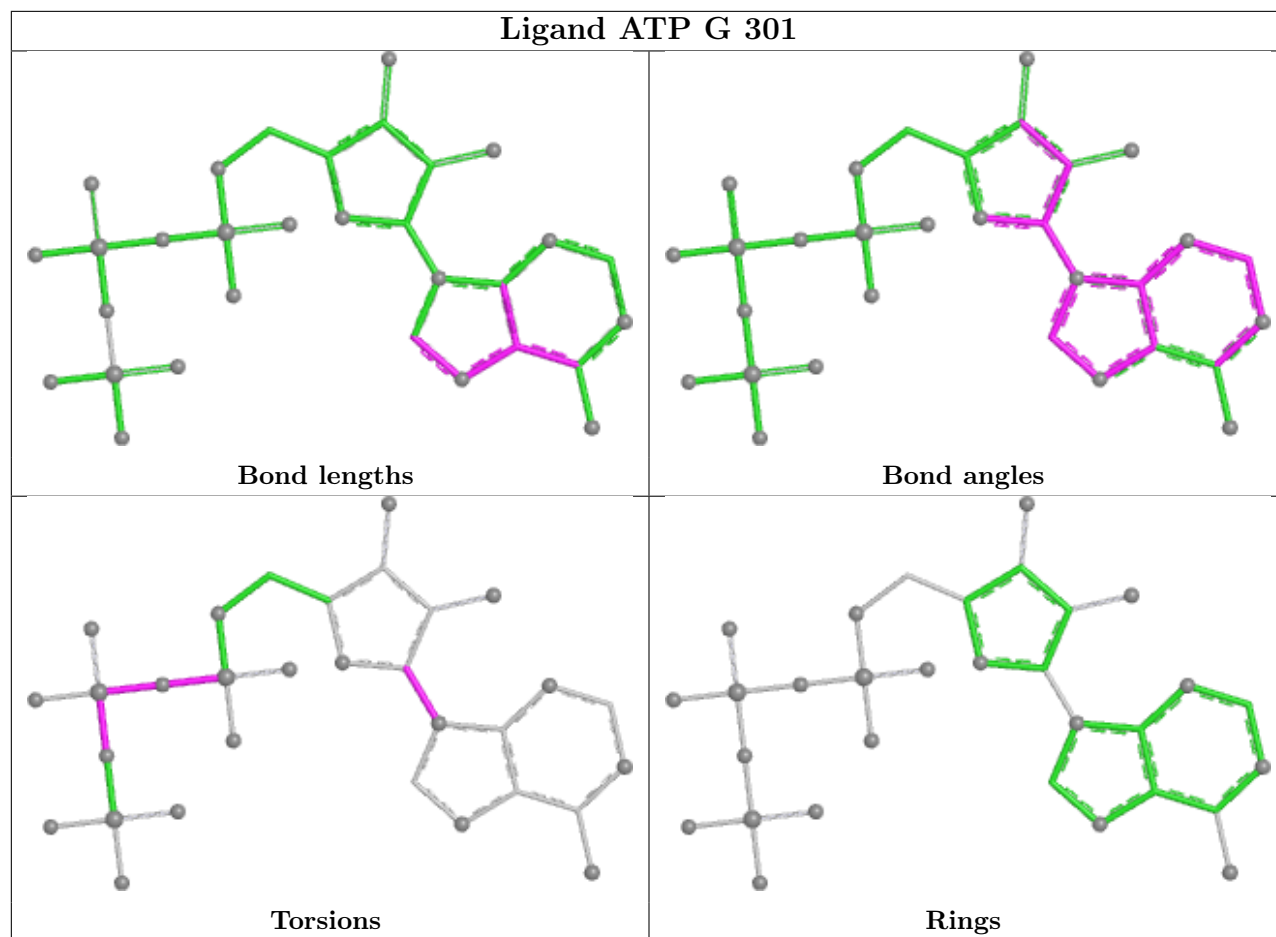
| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 9   | G     | 301    | ATP  | 2       | 0            |
| 6   | B     | 304[A] | MOO  | 4       | 0            |
| 5   | L     | 303    | 8M0  | 5       | 0            |
| 5   | K     | 303    | 8M0  | 2       | 0            |
| 5   | I     | 303    | 8M0  | 1       | 0            |
| 9   | E     | 301    | ATP  | 2       | 0            |
| 6   | J     | 304[A] | MOO  | 4       | 0            |
| 5   | F     | 303    | 8M0  | 6       | 0            |
| 9   | C     | 302    | ATP  | 1       | 0            |
| 9   | I     | 301    | ATP  | 2       | 0            |
| 9   | K     | 301    | ATP  | 1       | 0            |
| 5   | B     | 303    | 8M0  | 4       | 0            |
| 5   | C     | 301    | 8M0  | 3       | 0            |
| 9   | A     | 301    | ATP  | 1       | 0            |
| 5   | C     | 304    | 8M0  | 1       | 0            |
| 6   | H     | 304[A] | MOO  | 4       | 0            |

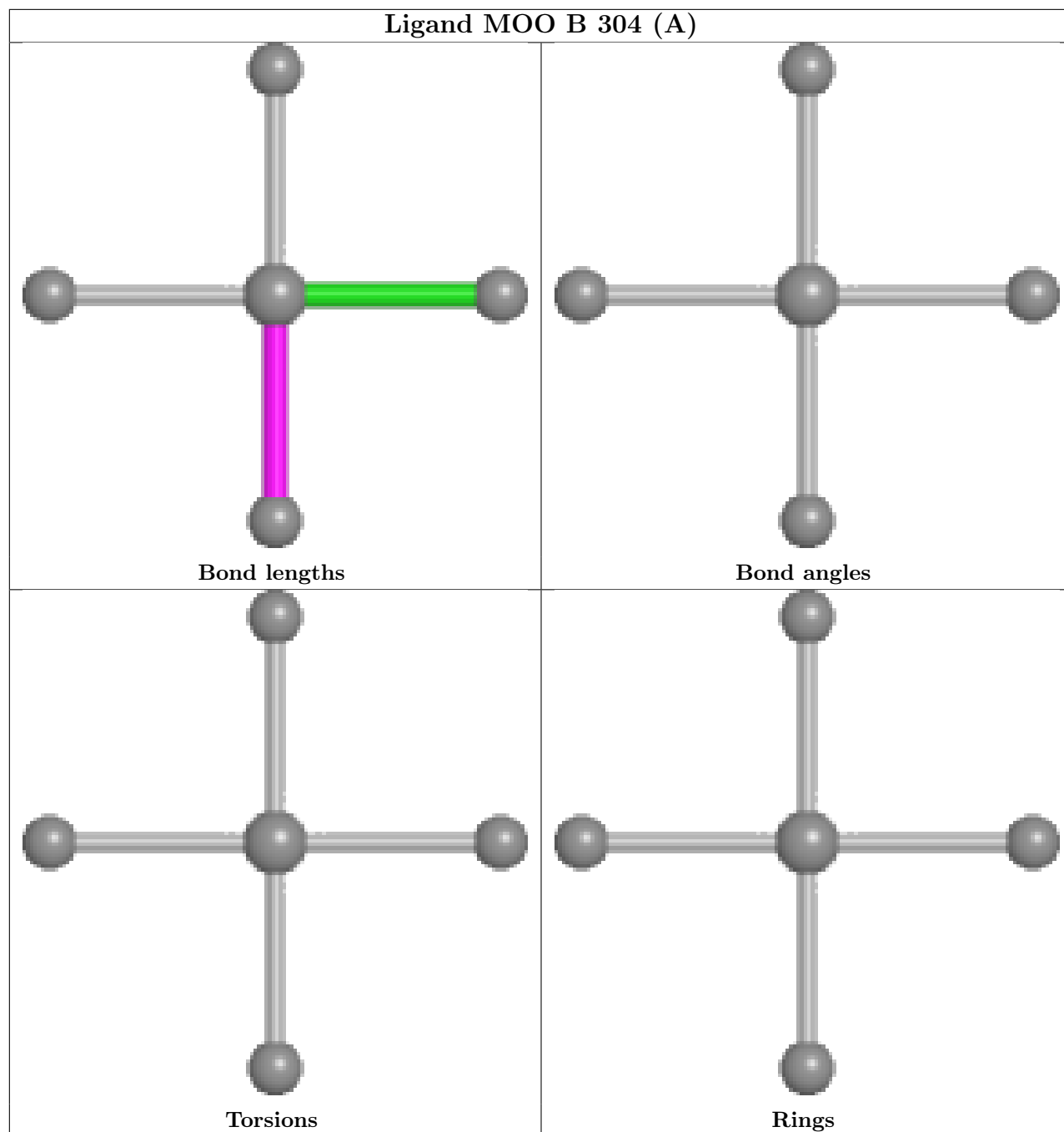
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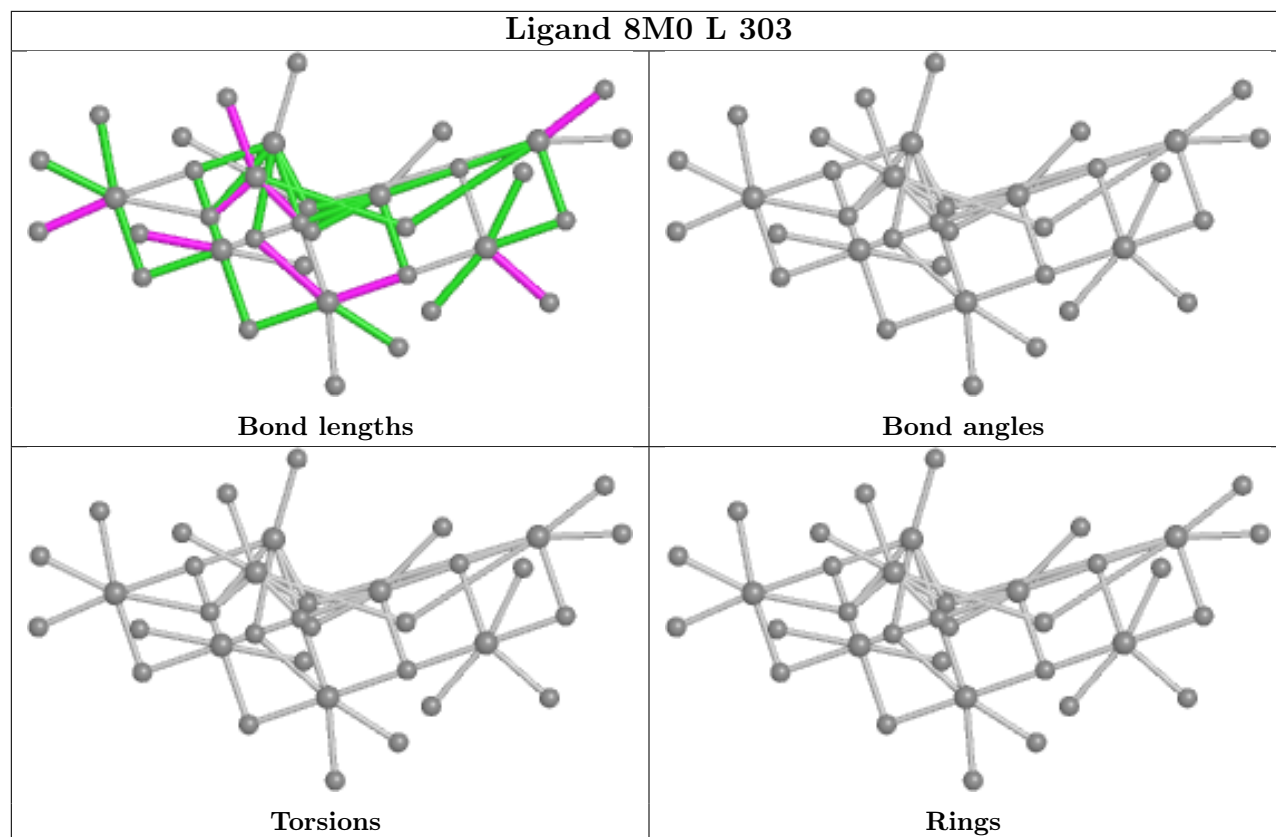
| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 5   | A     | 303    | 8M0  | 1       | 0            |
| 6   | F     | 304[A] | MOO  | 4       | 0            |
| 10  | G     | 304    | M10  | 3       | 0            |
| 5   | J     | 302    | 8M0  | 2       | 0            |
| 10  | A     | 304    | M10  | 3       | 0            |
| 6   | D     | 303[A] | MOO  | 4       | 0            |
| 5   | H     | 303    | 8M0  | 2       | 0            |
| 5   | G     | 303    | 8M0  | 1       | 0            |
| 6   | L     | 304[A] | MOO  | 4       | 0            |
| 5   | E     | 303    | 8M0  | 1       | 0            |
| 3   | B     | 301    | ADP  | 1       | 0            |

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

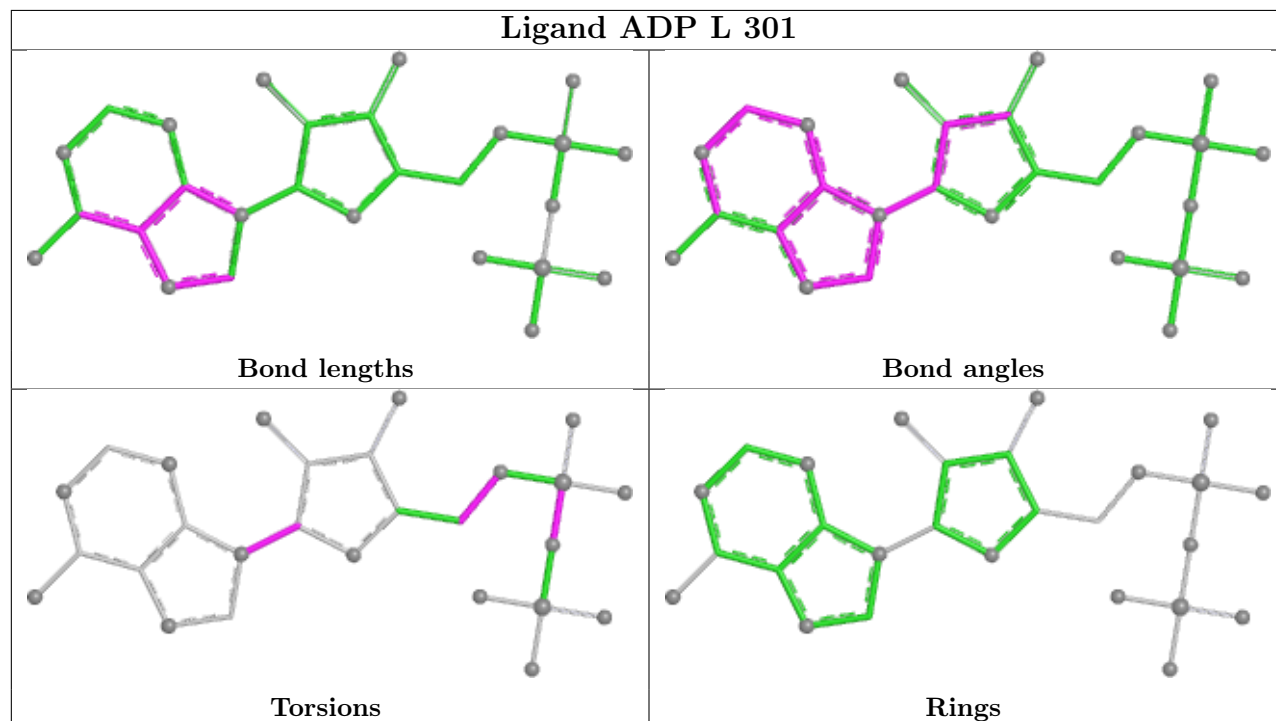




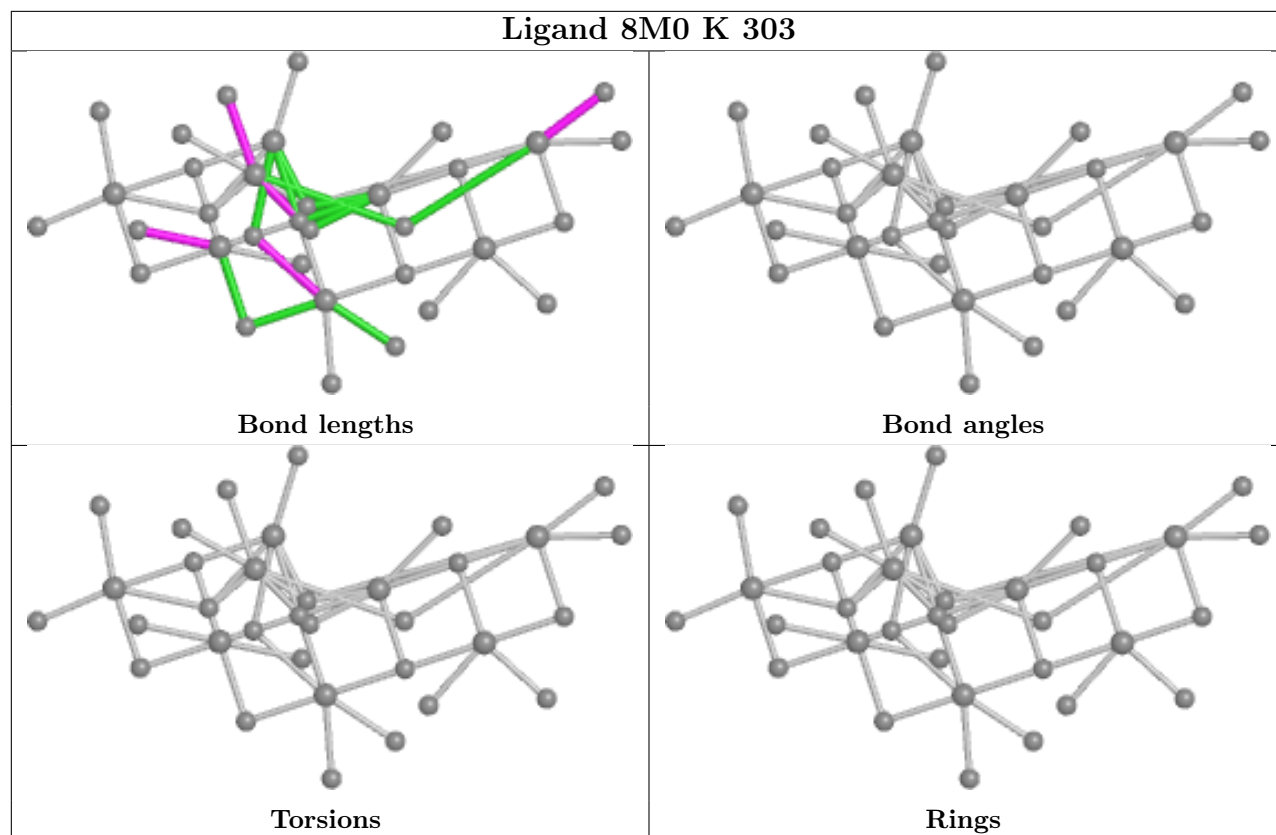
## Ligand 8M0 L 303



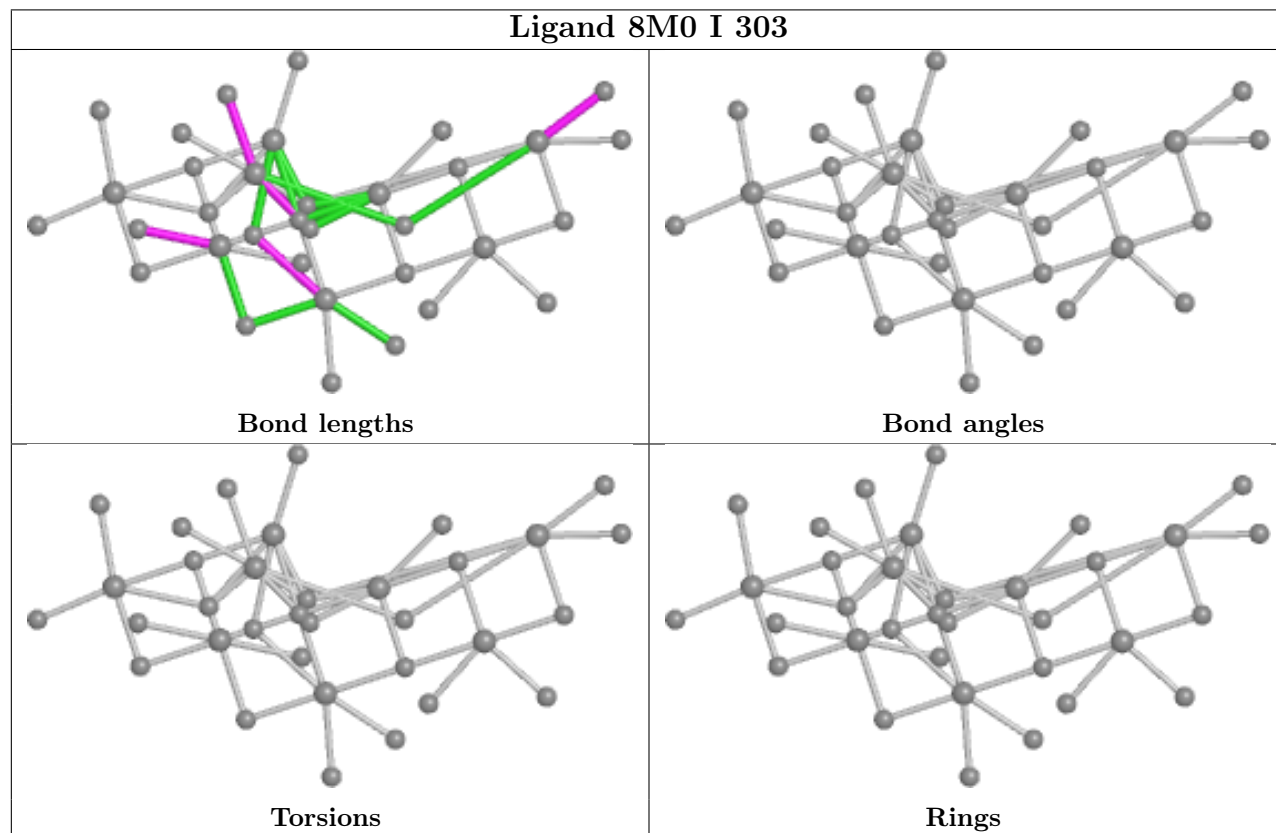
## Ligand ADP L 301

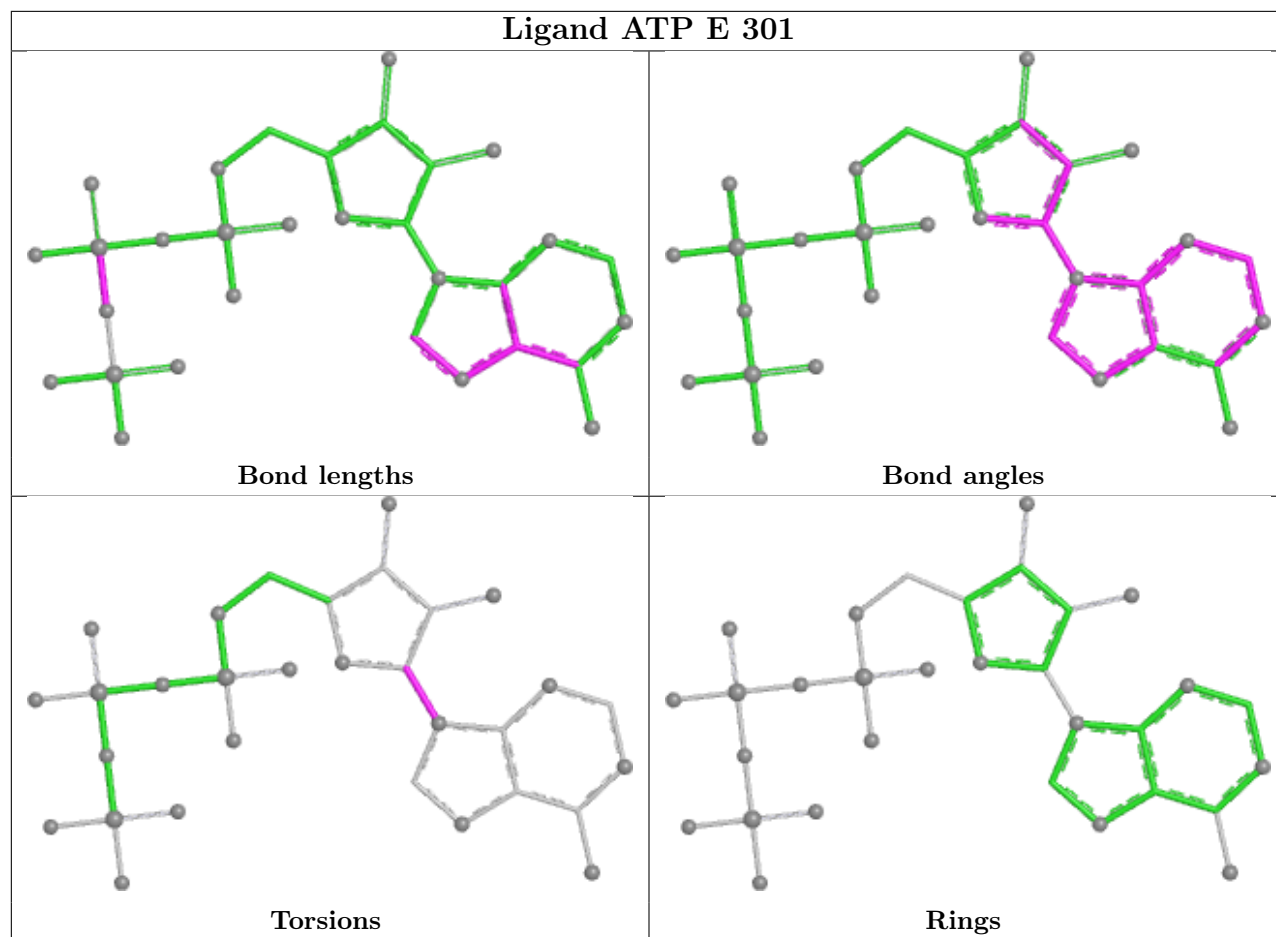


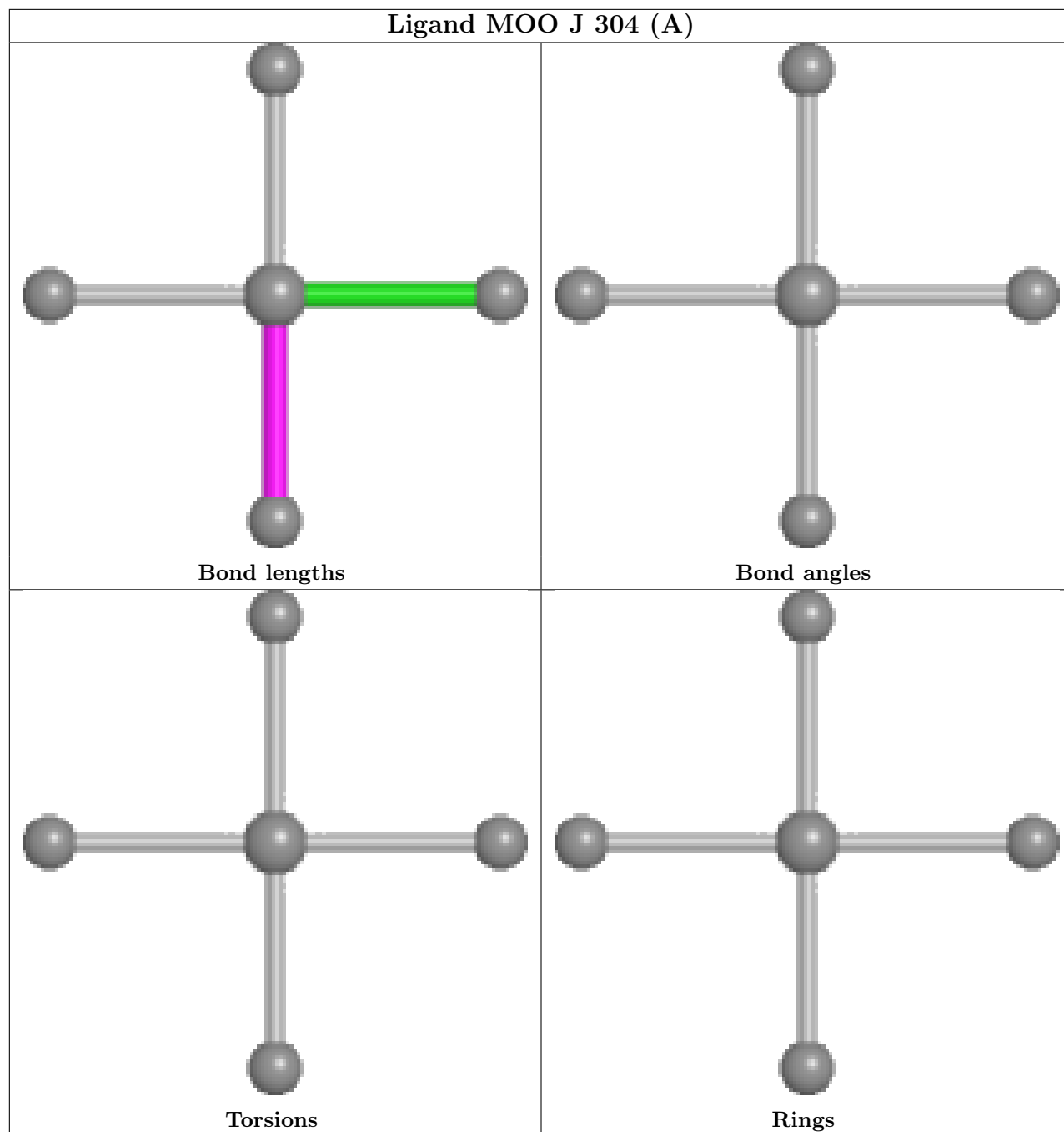
## Ligand 8M0 K 303



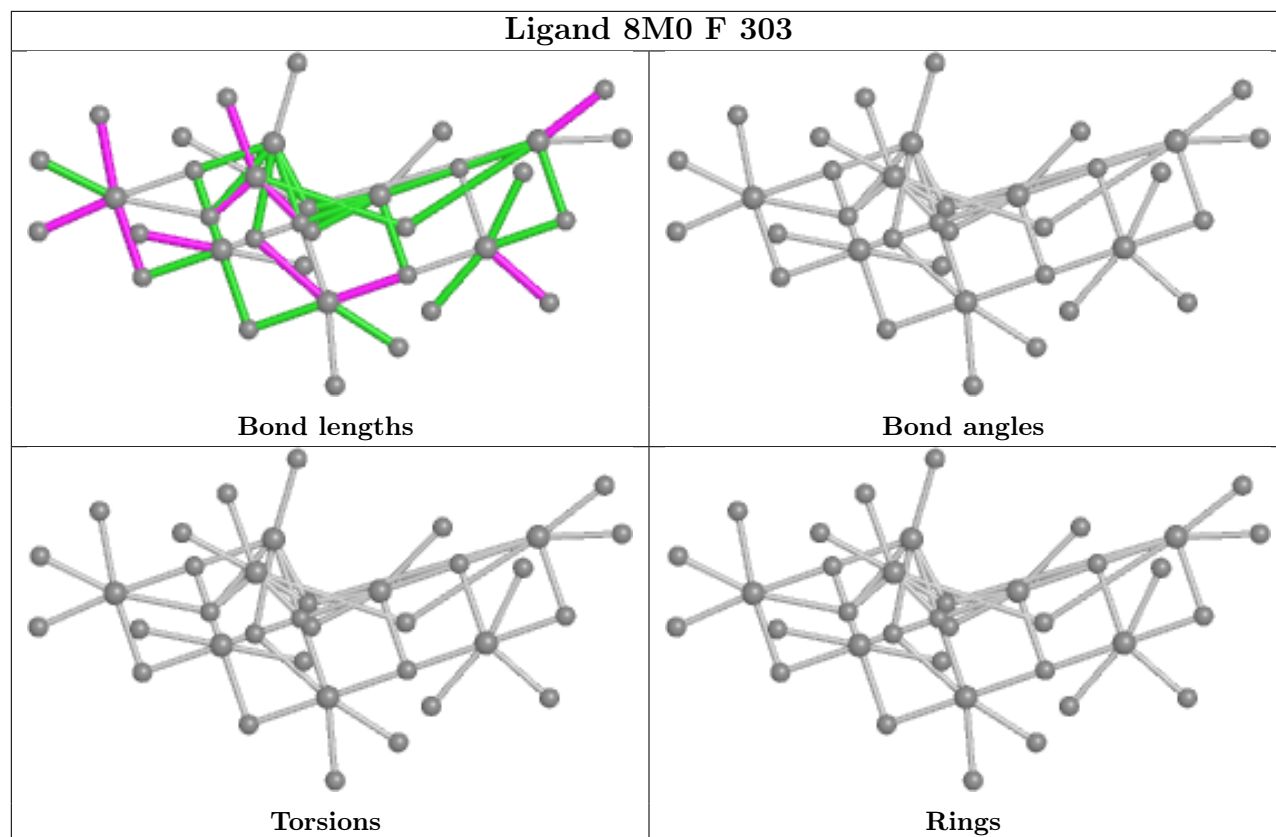
## Ligand 8M0 I 303



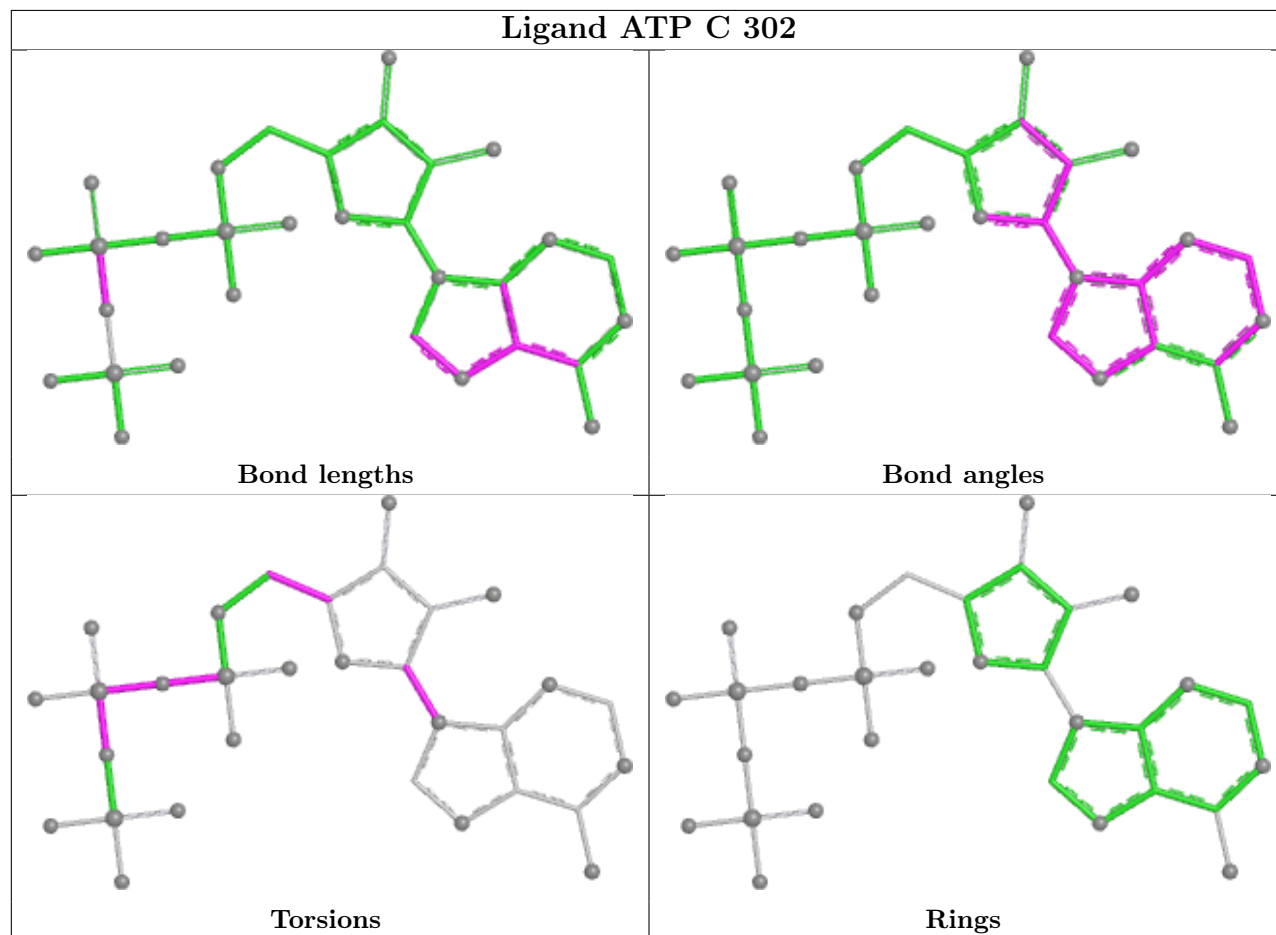


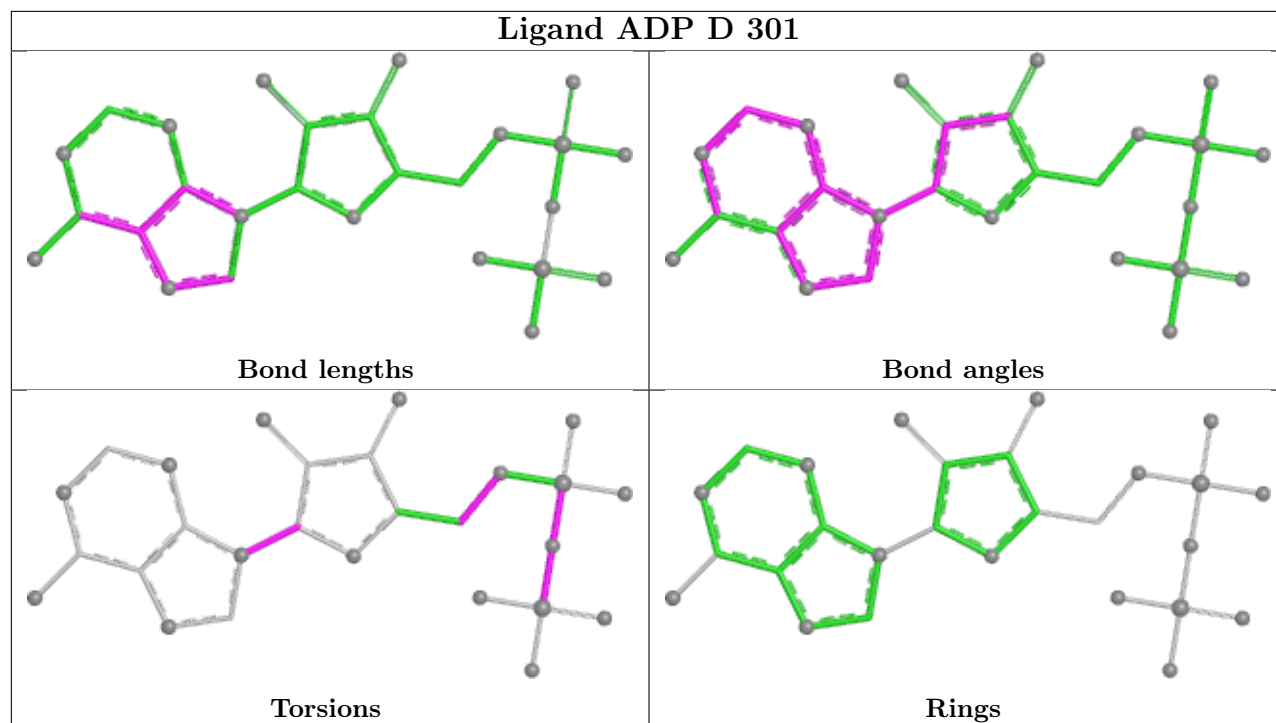


## Ligand 8M0 F 303

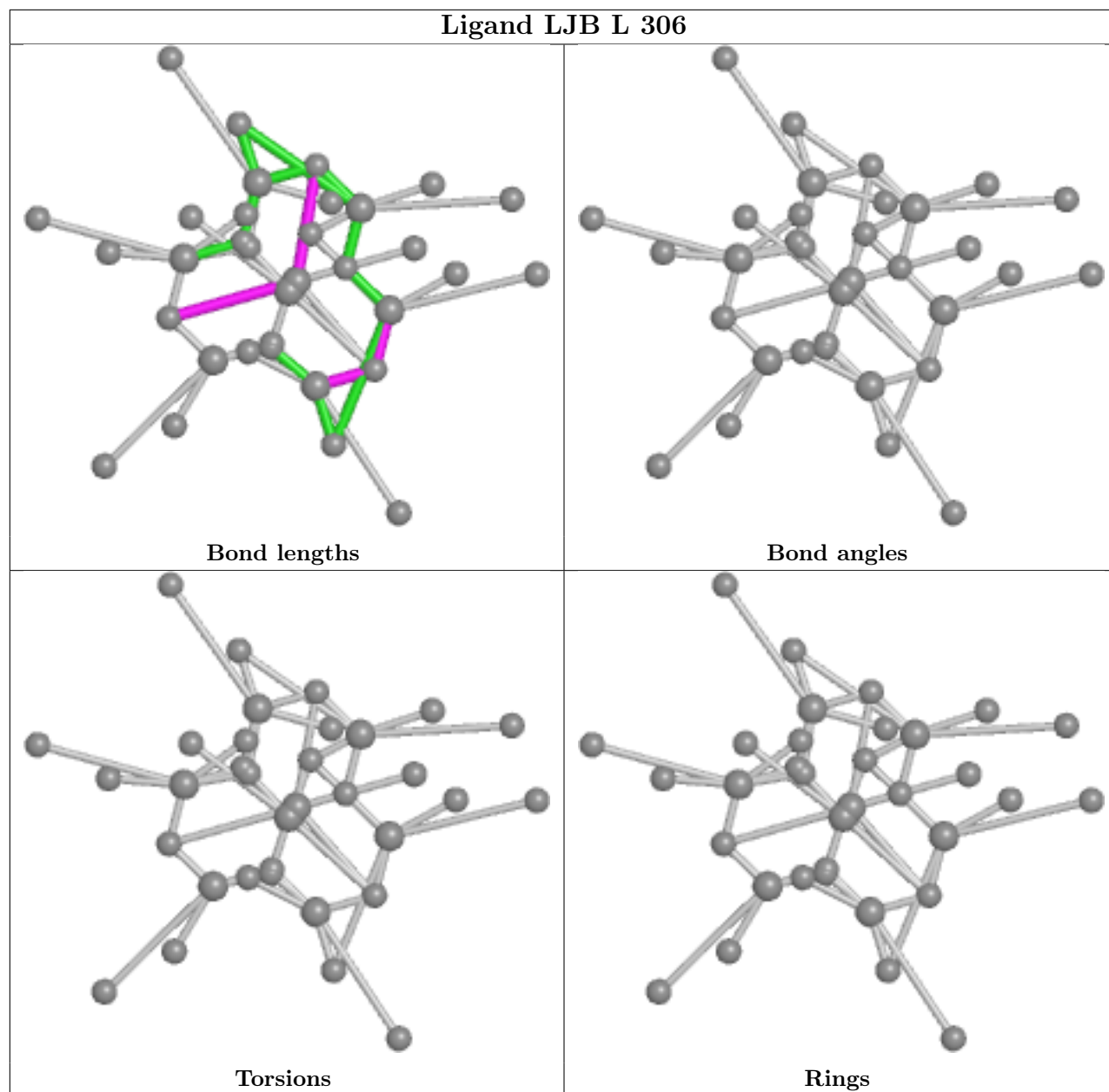


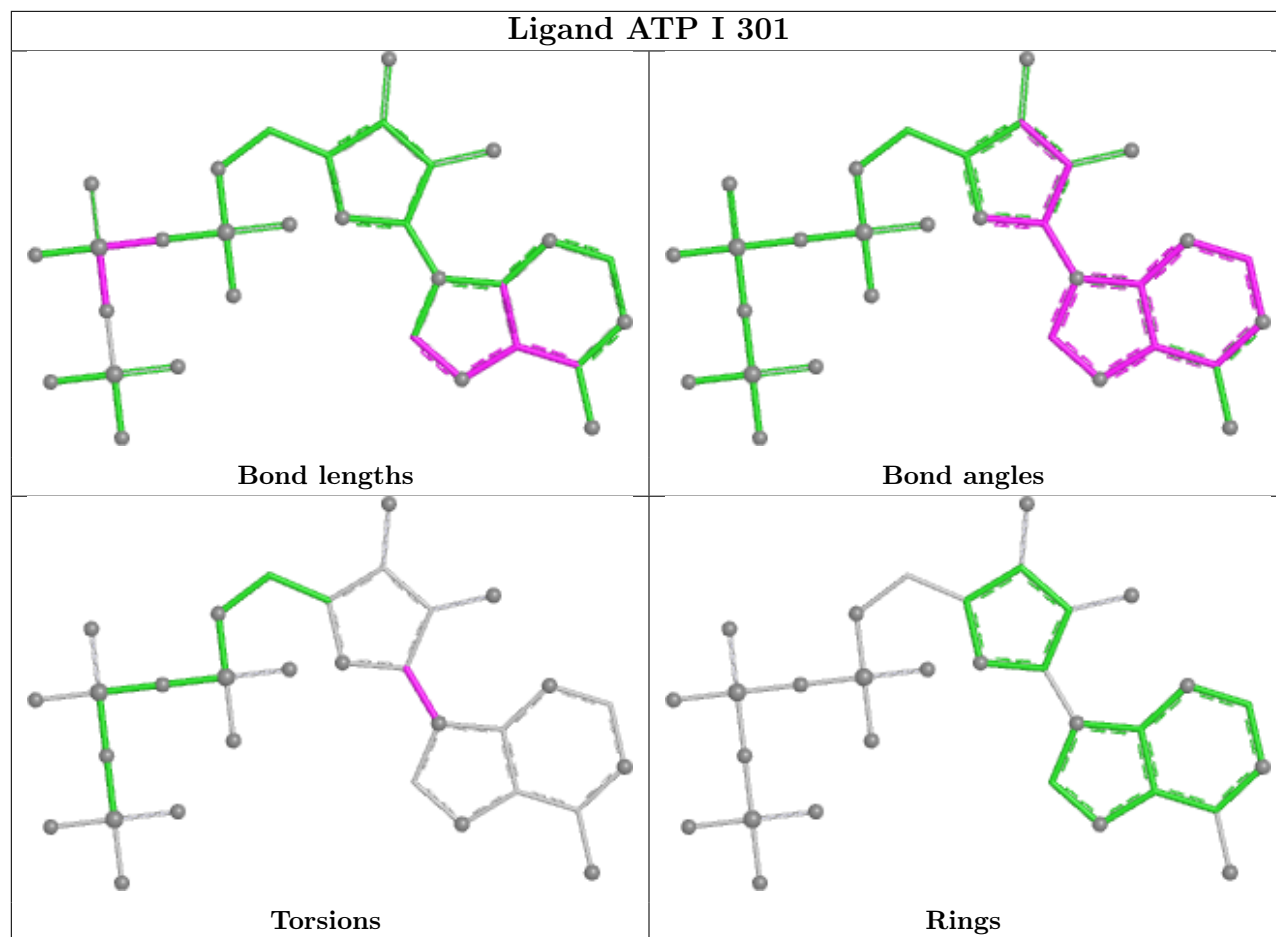
## Ligand ATP C 302



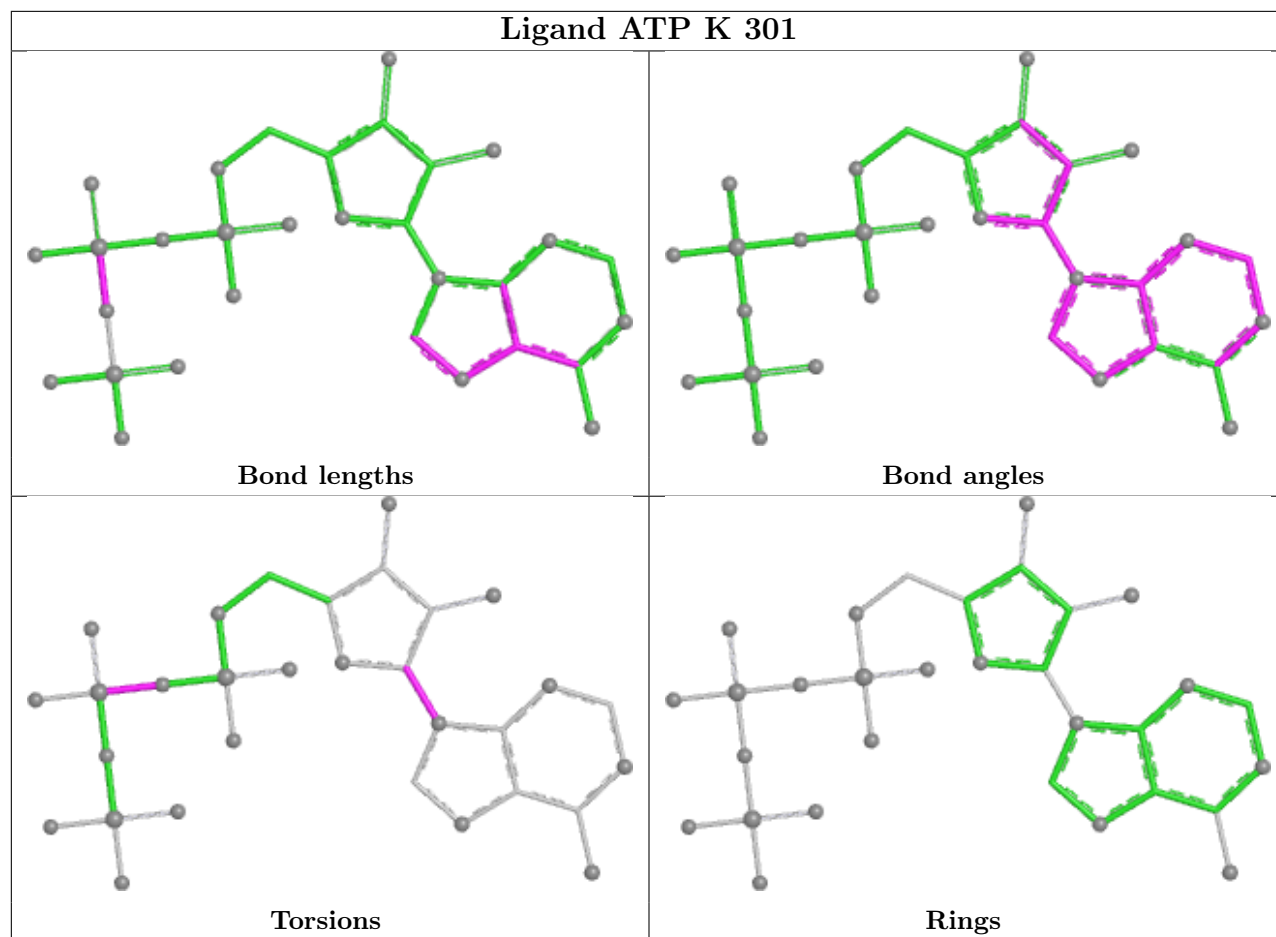


## Ligand LJB L 306

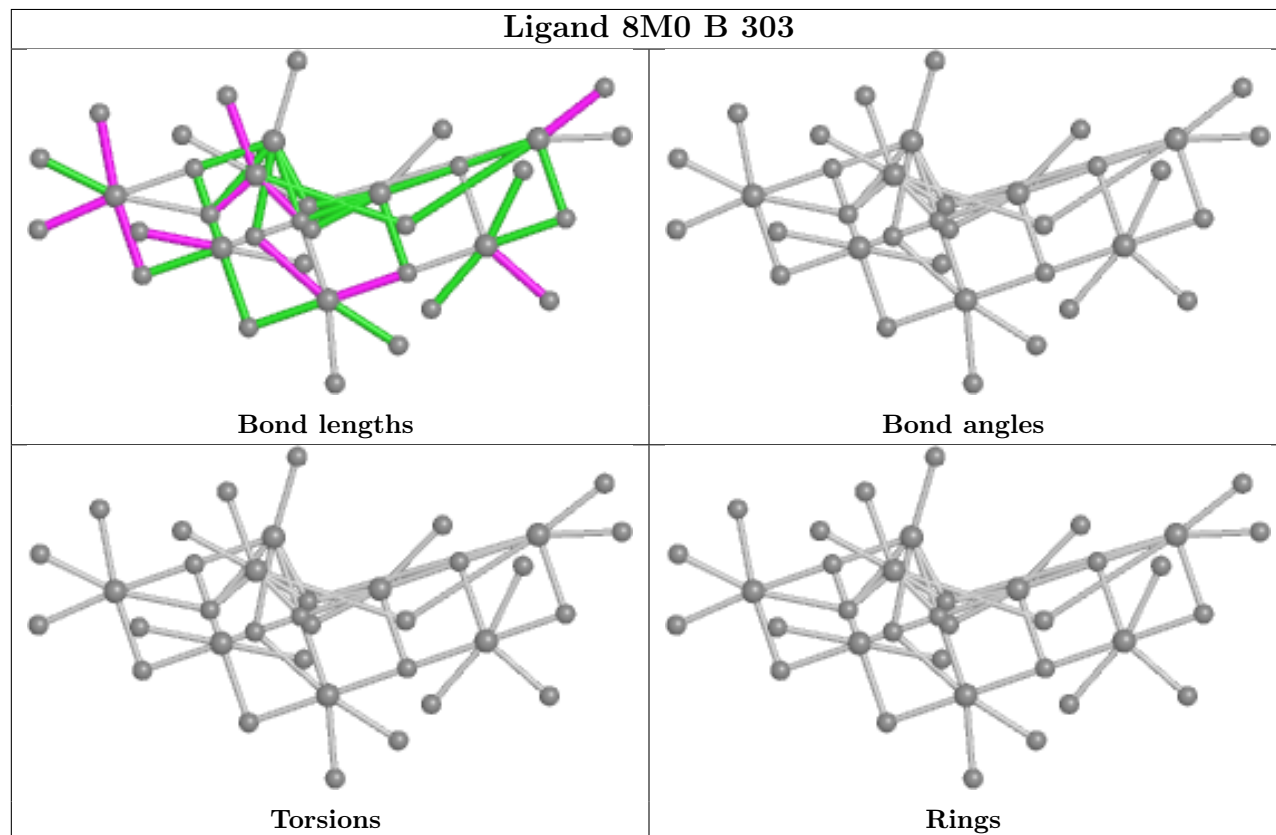




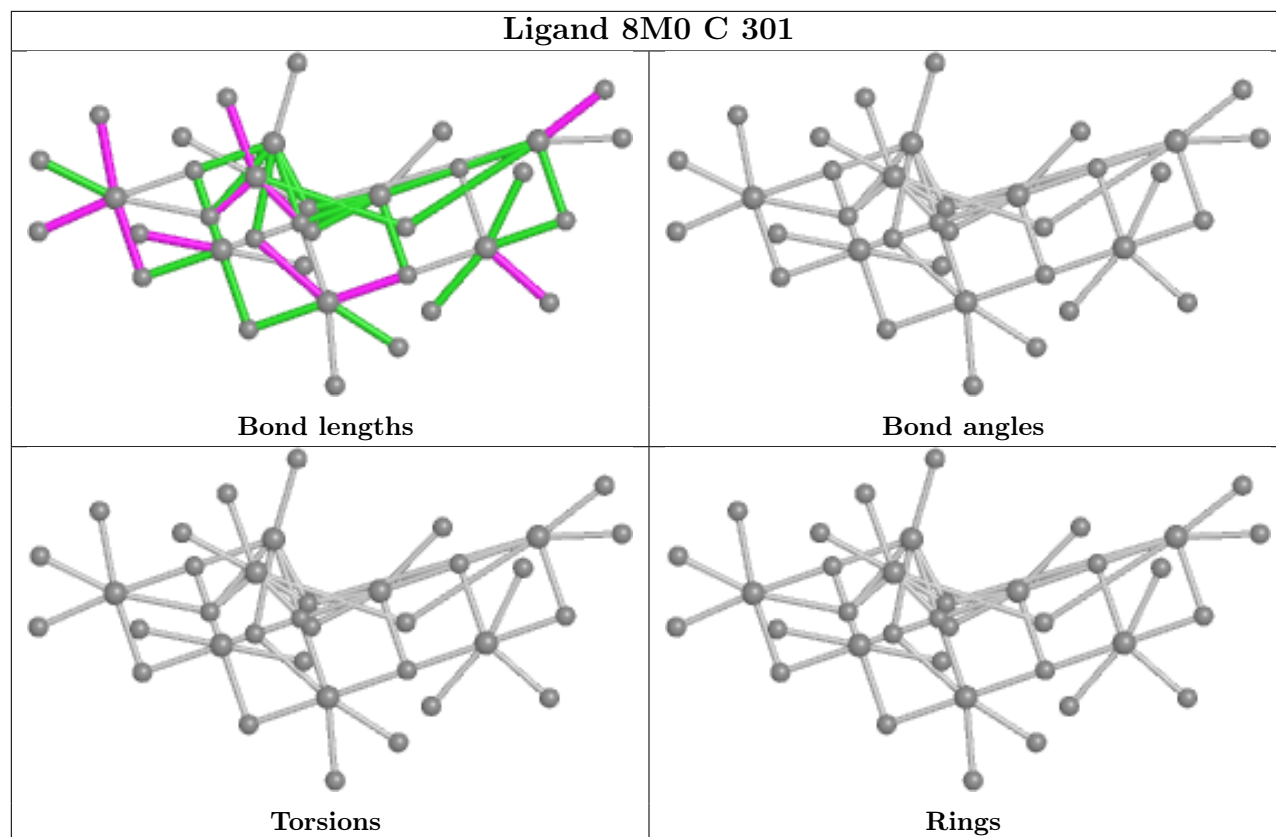
## Ligand ATP K 301



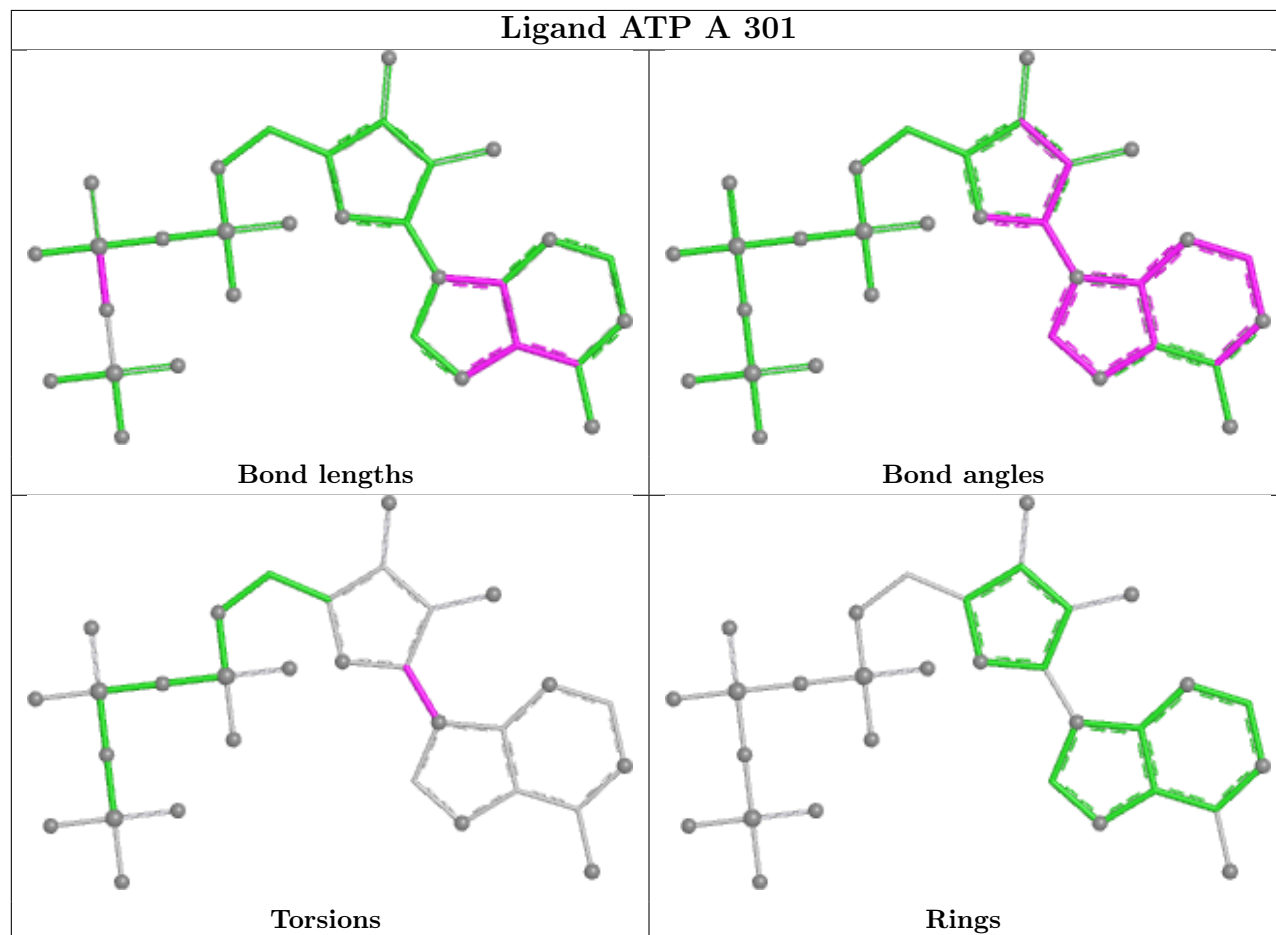
## Ligand 8M0 B 303

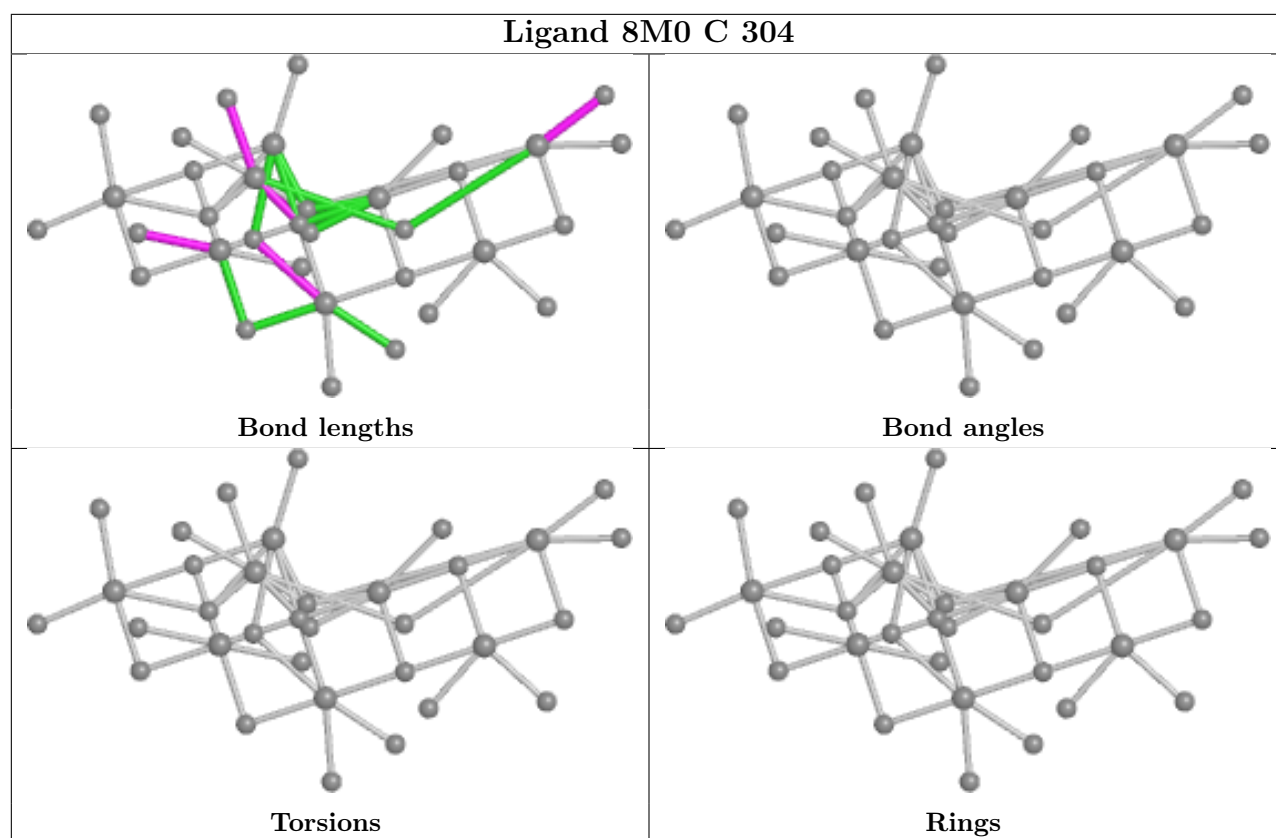


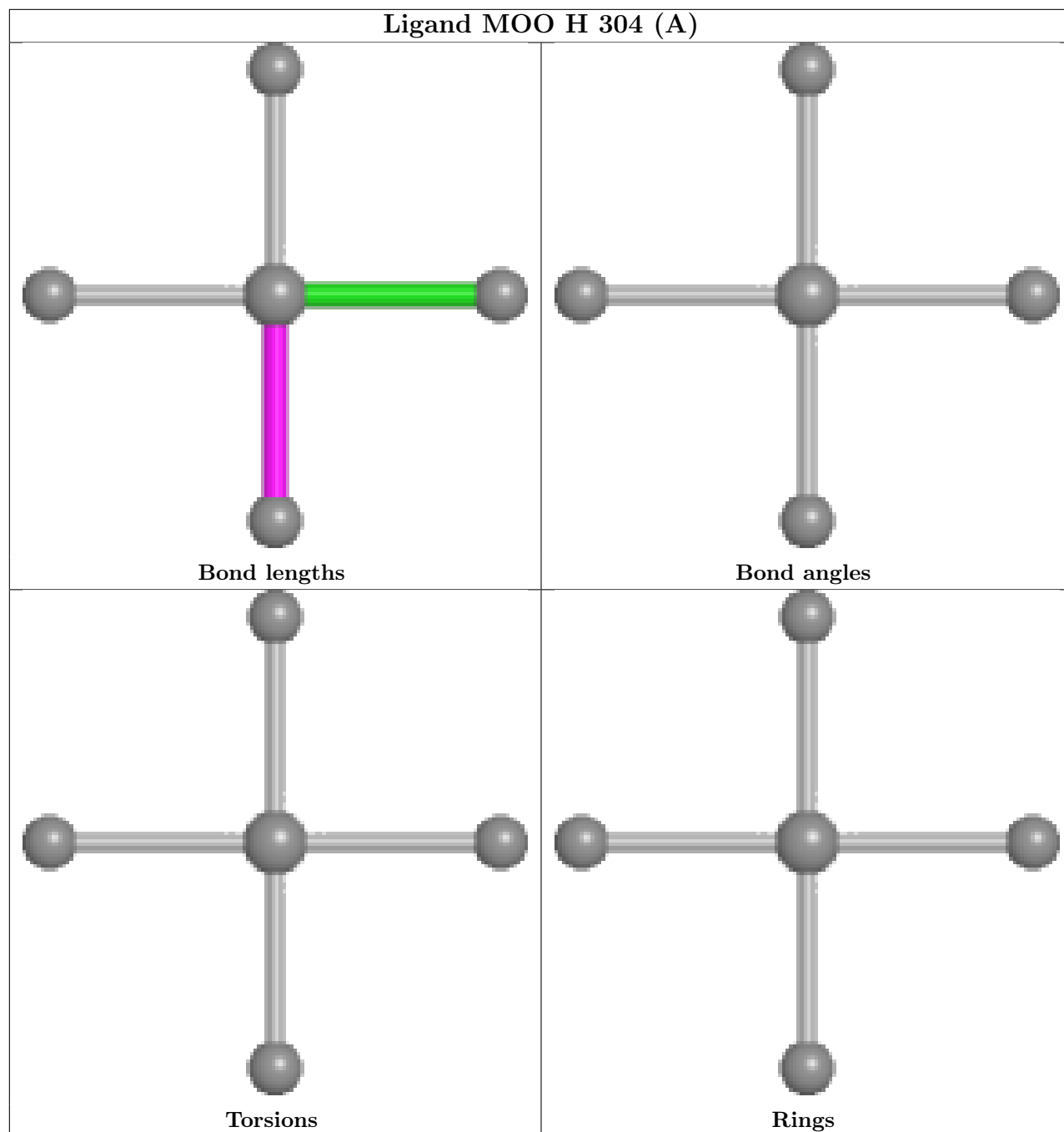
## Ligand 8M0 C 301



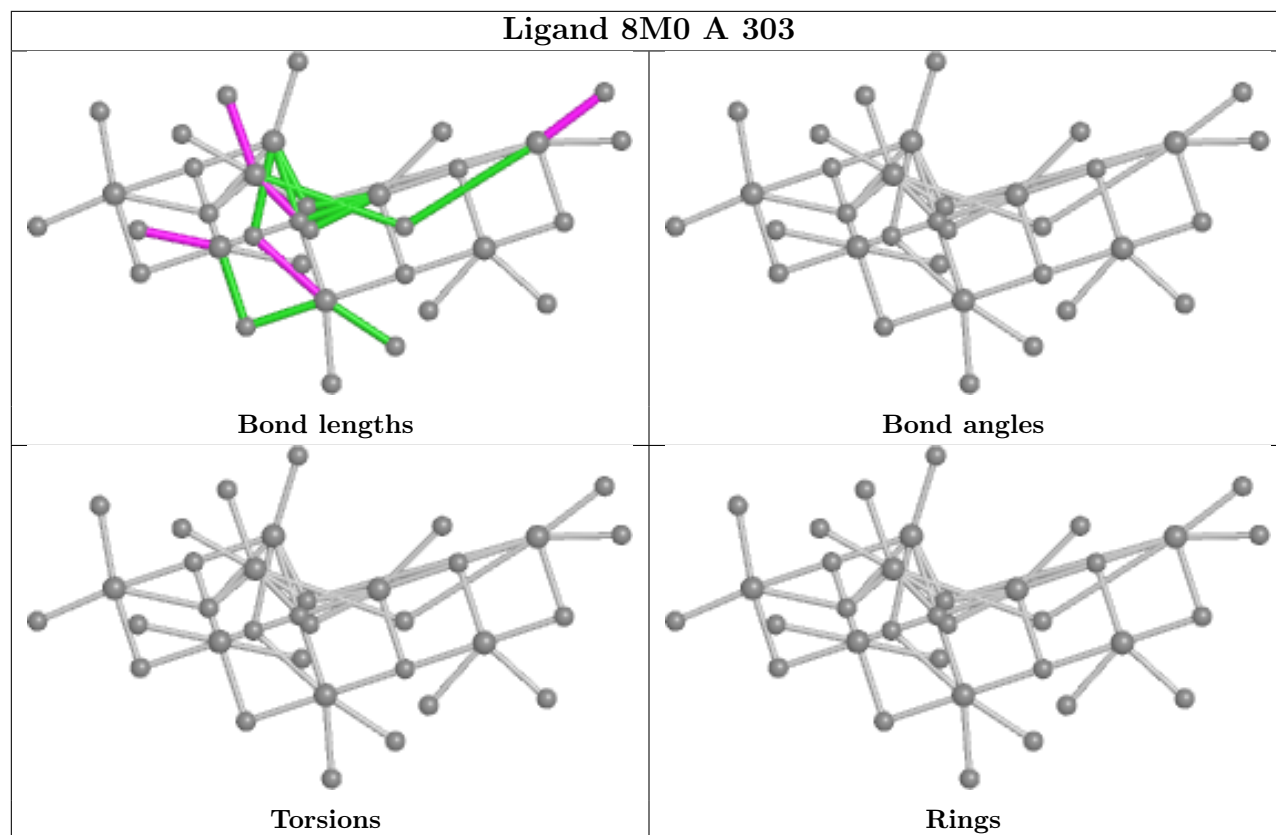
## Ligand ATP A 301

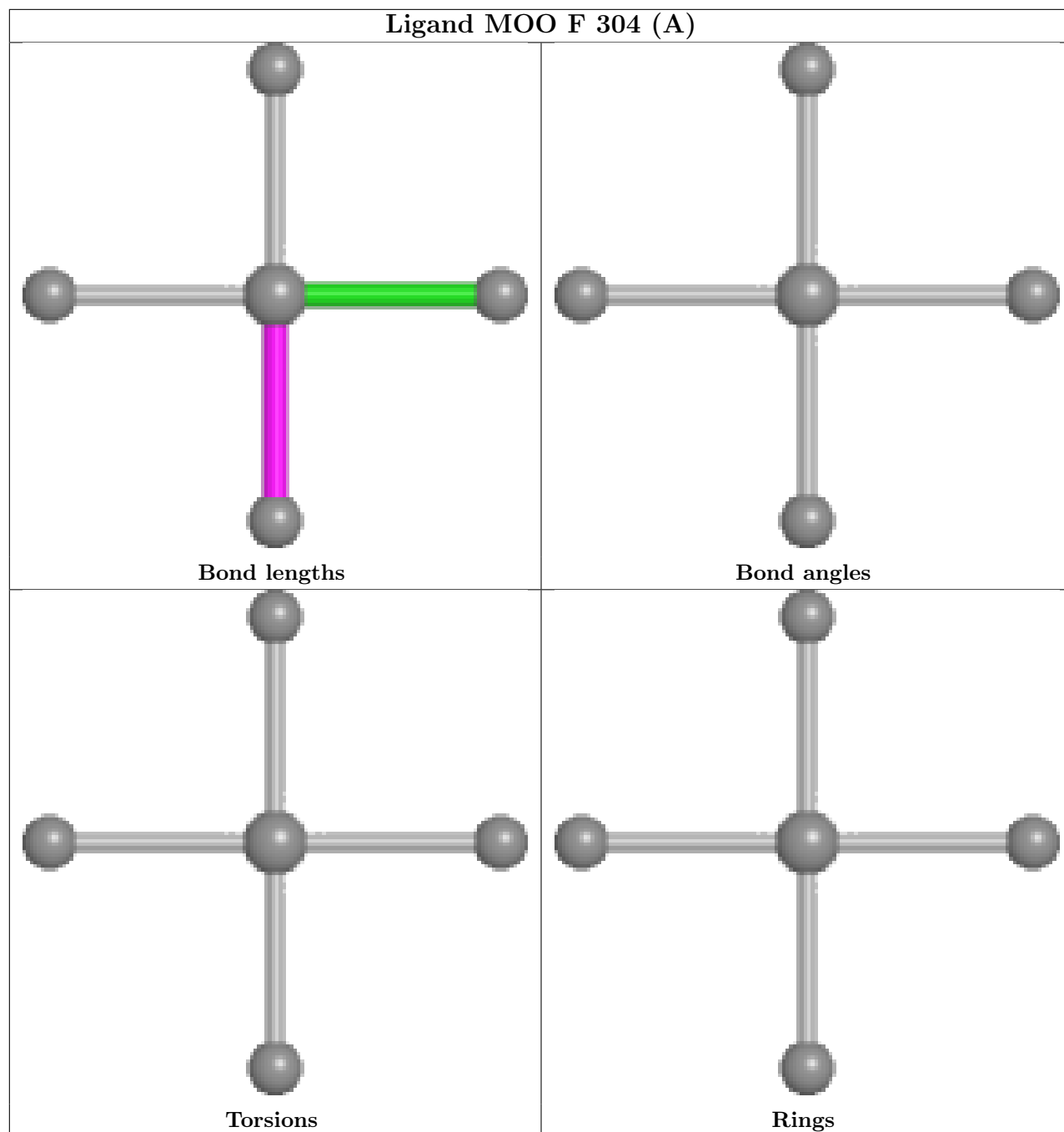




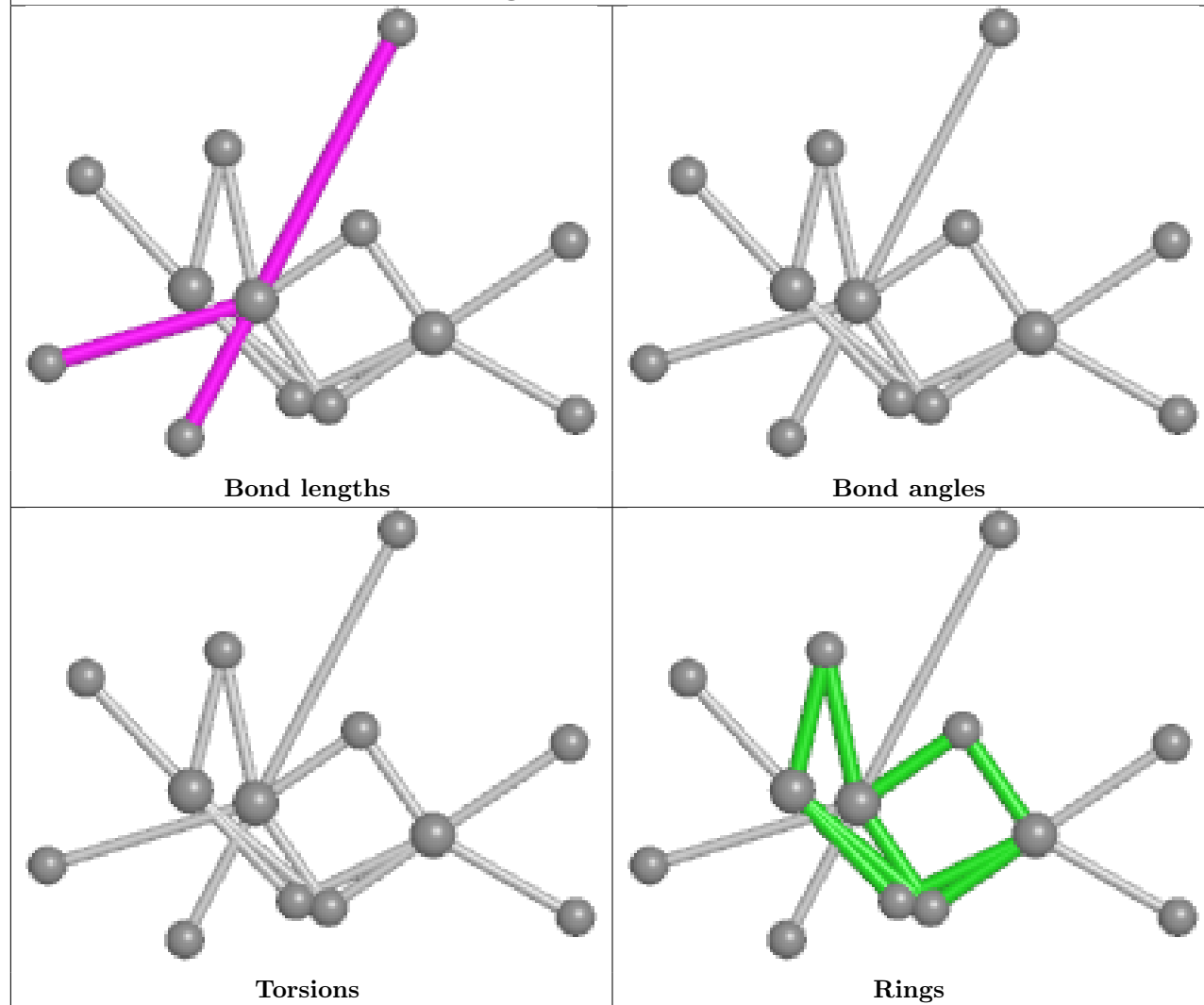


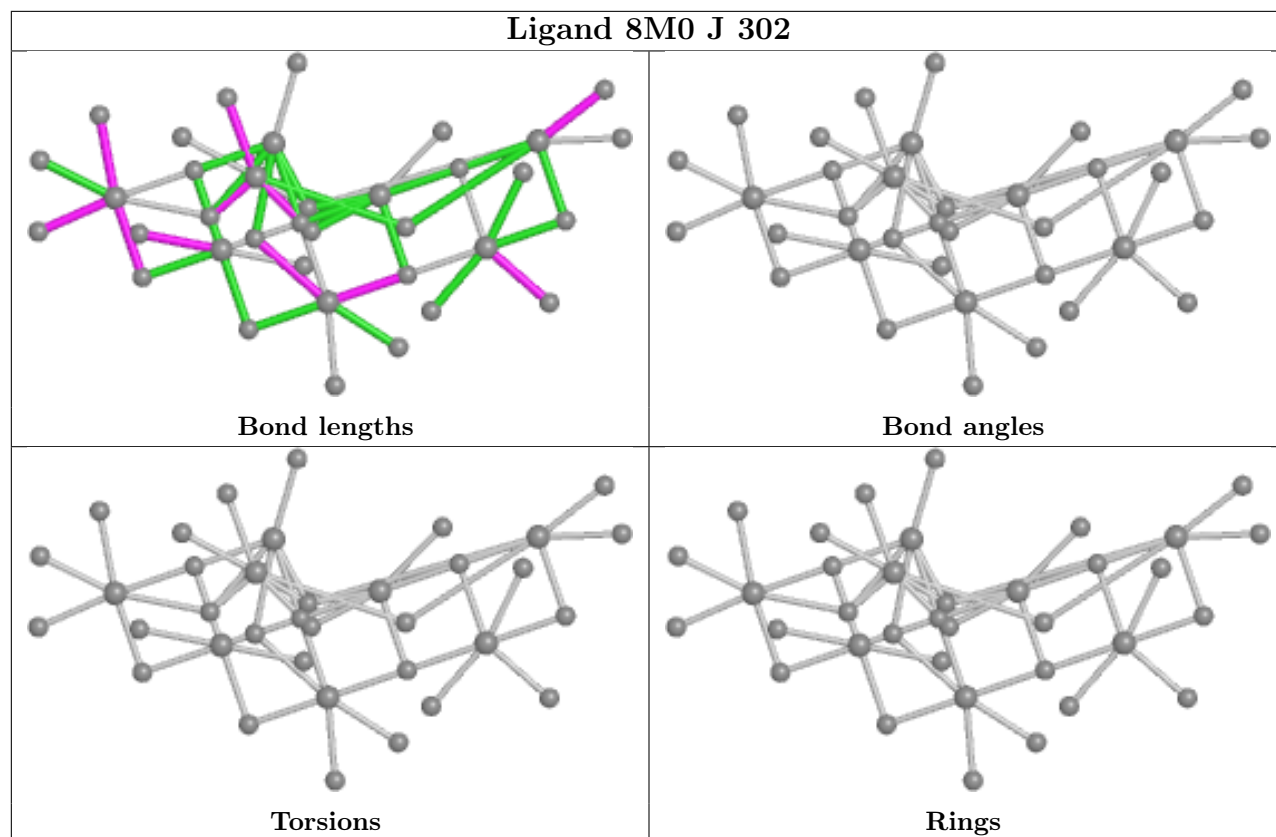
## Ligand 8M0 A 303

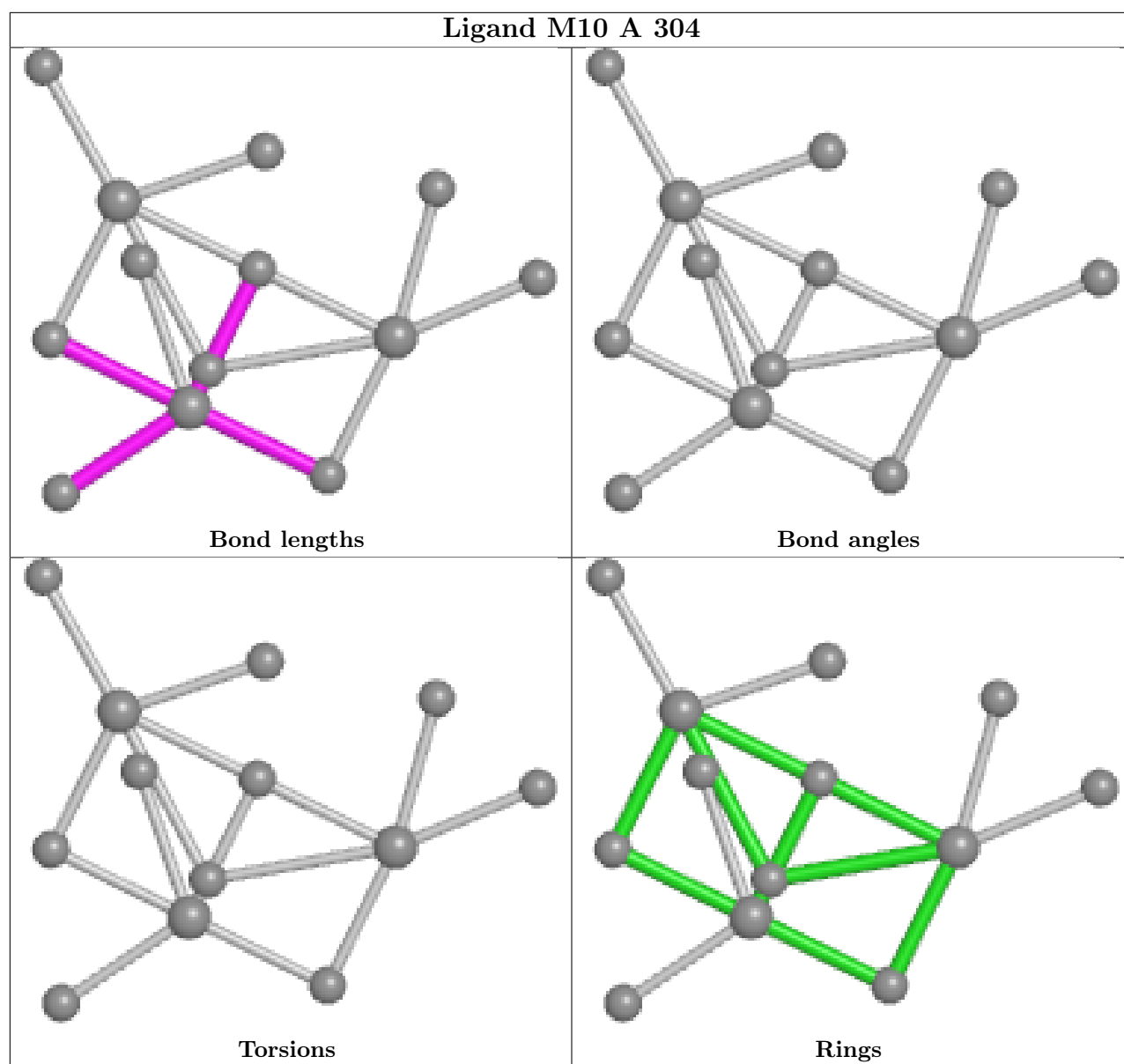


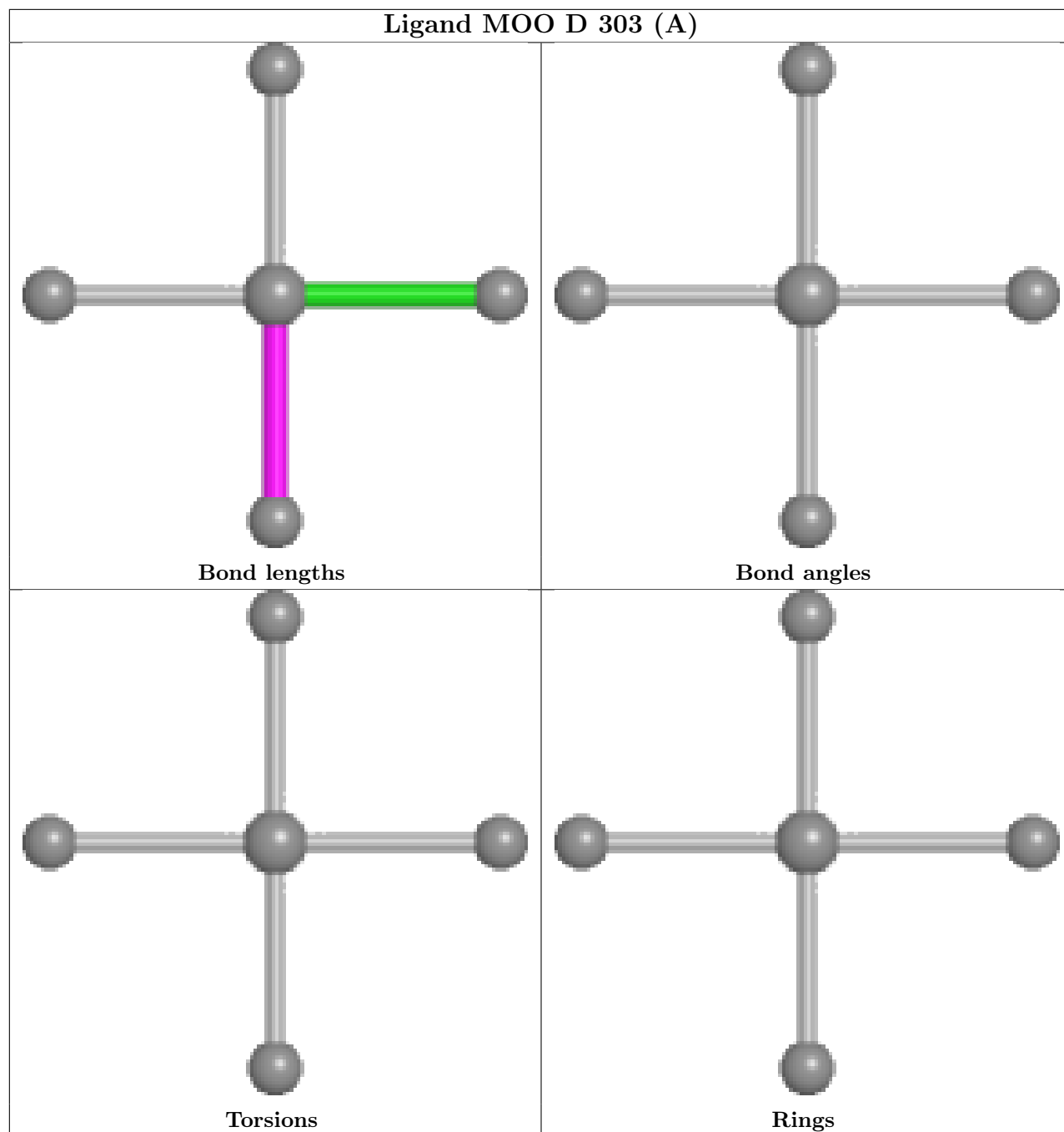


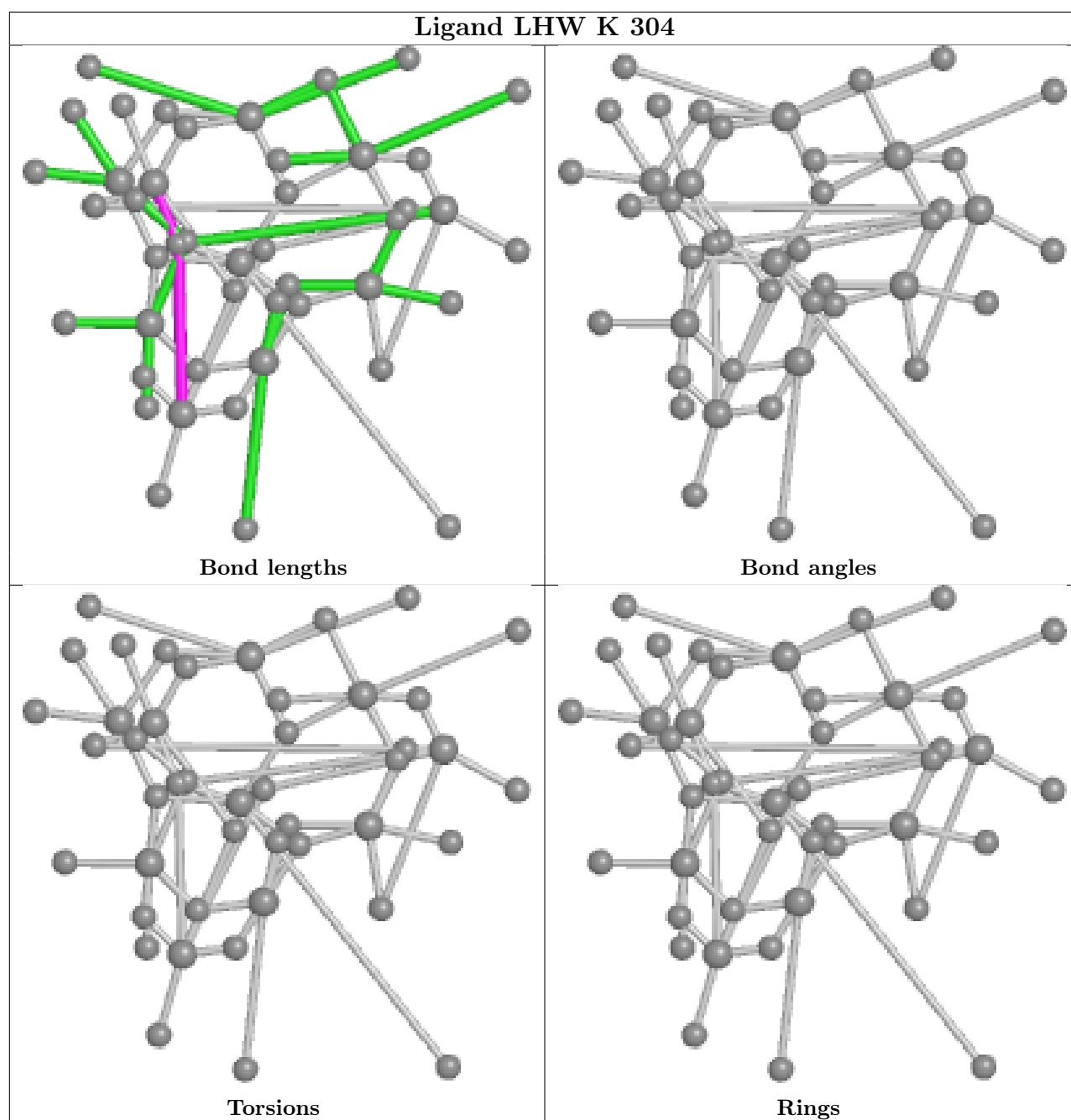
## Ligand M10 G 304



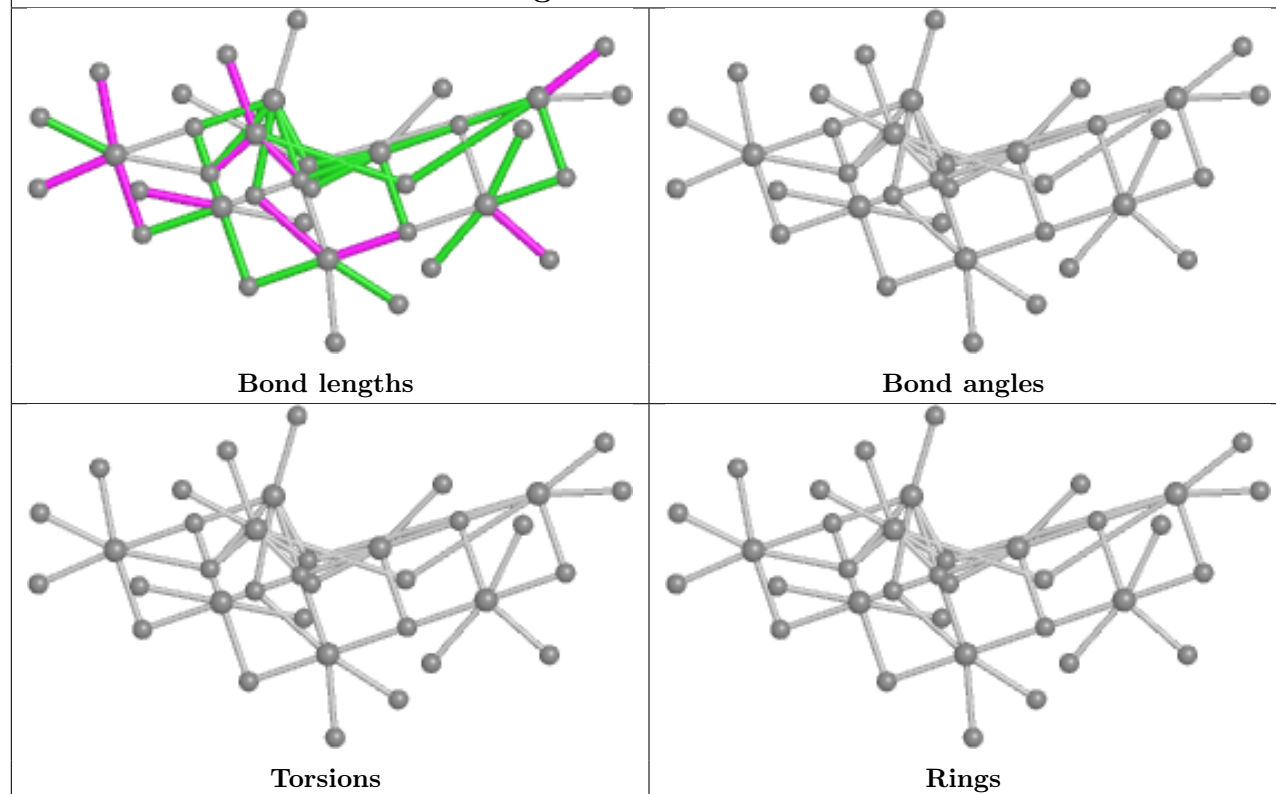




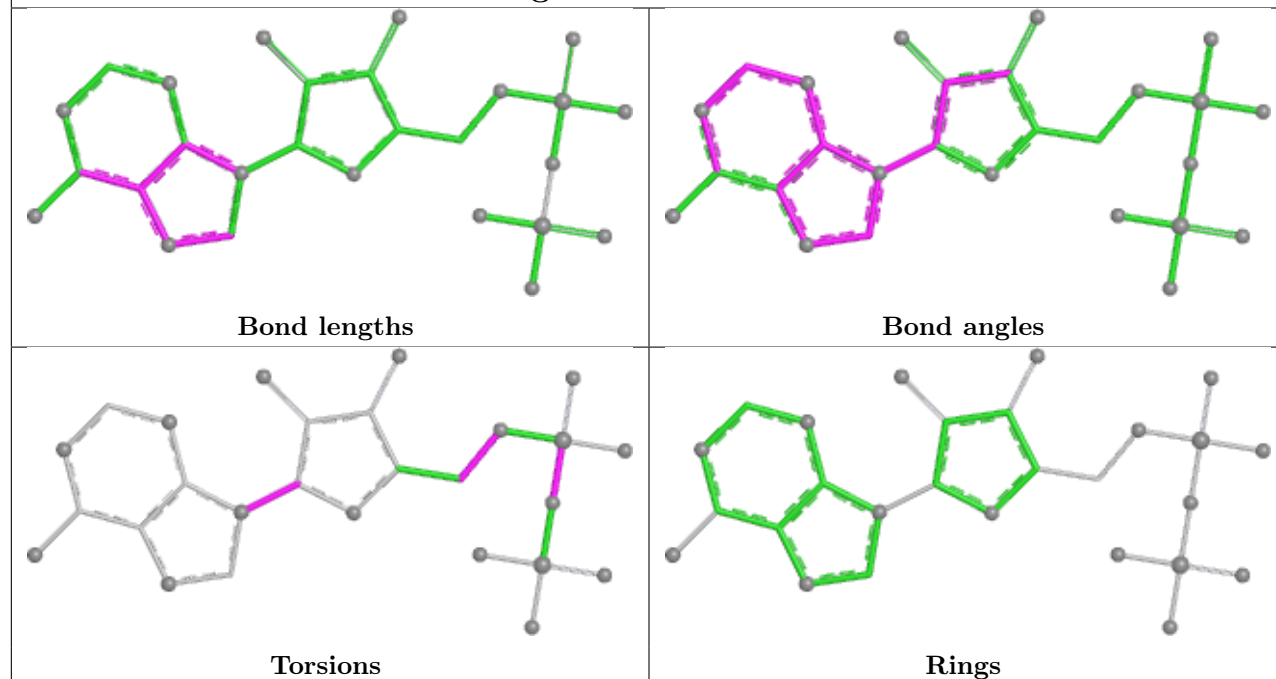


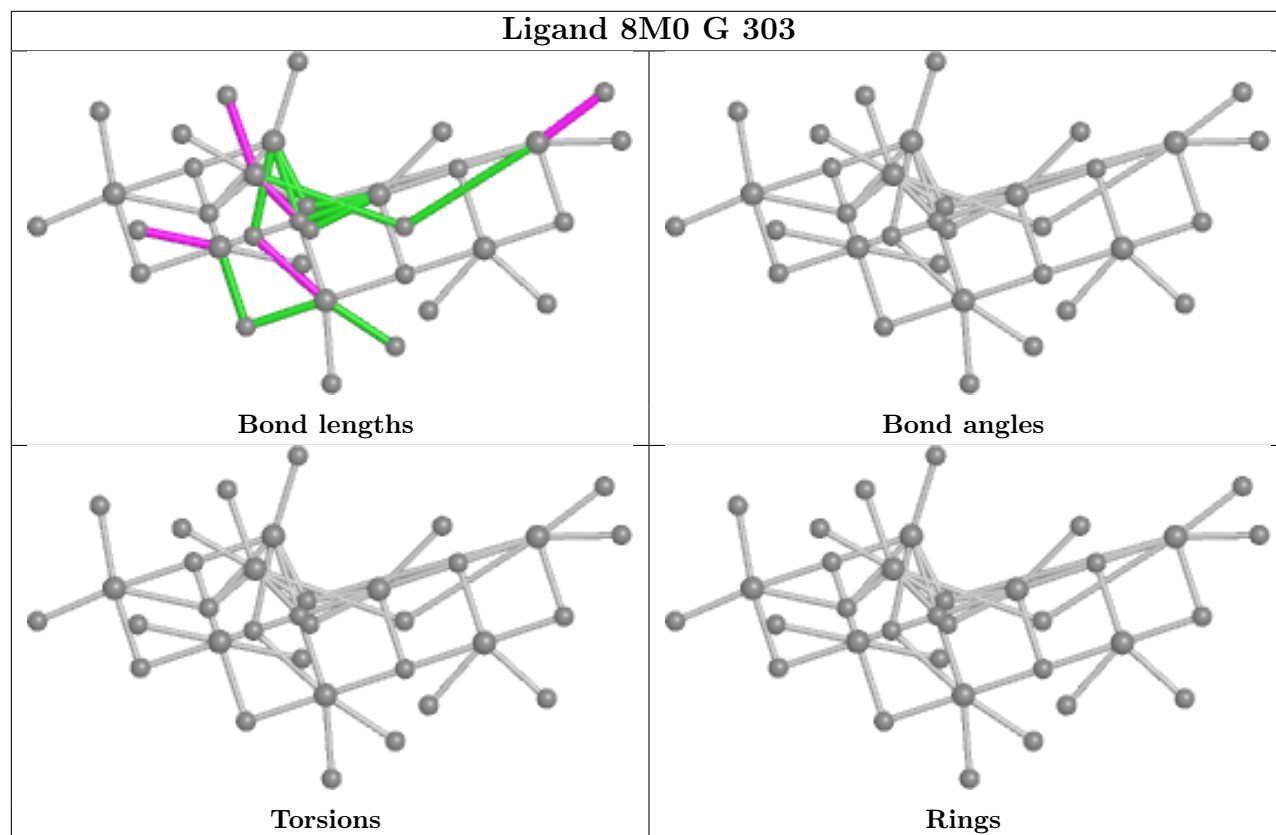


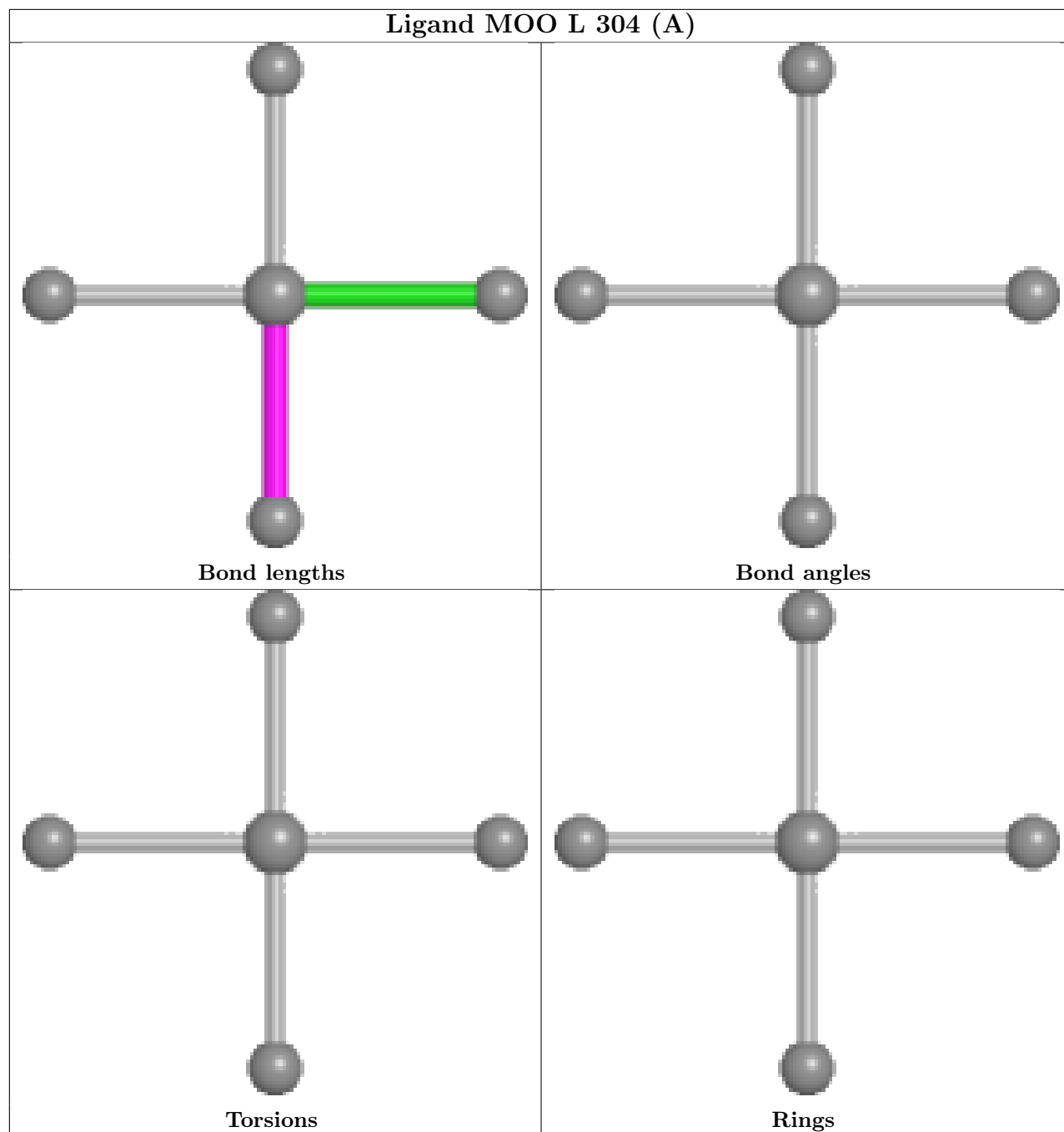
## Ligand 8M0 H 303

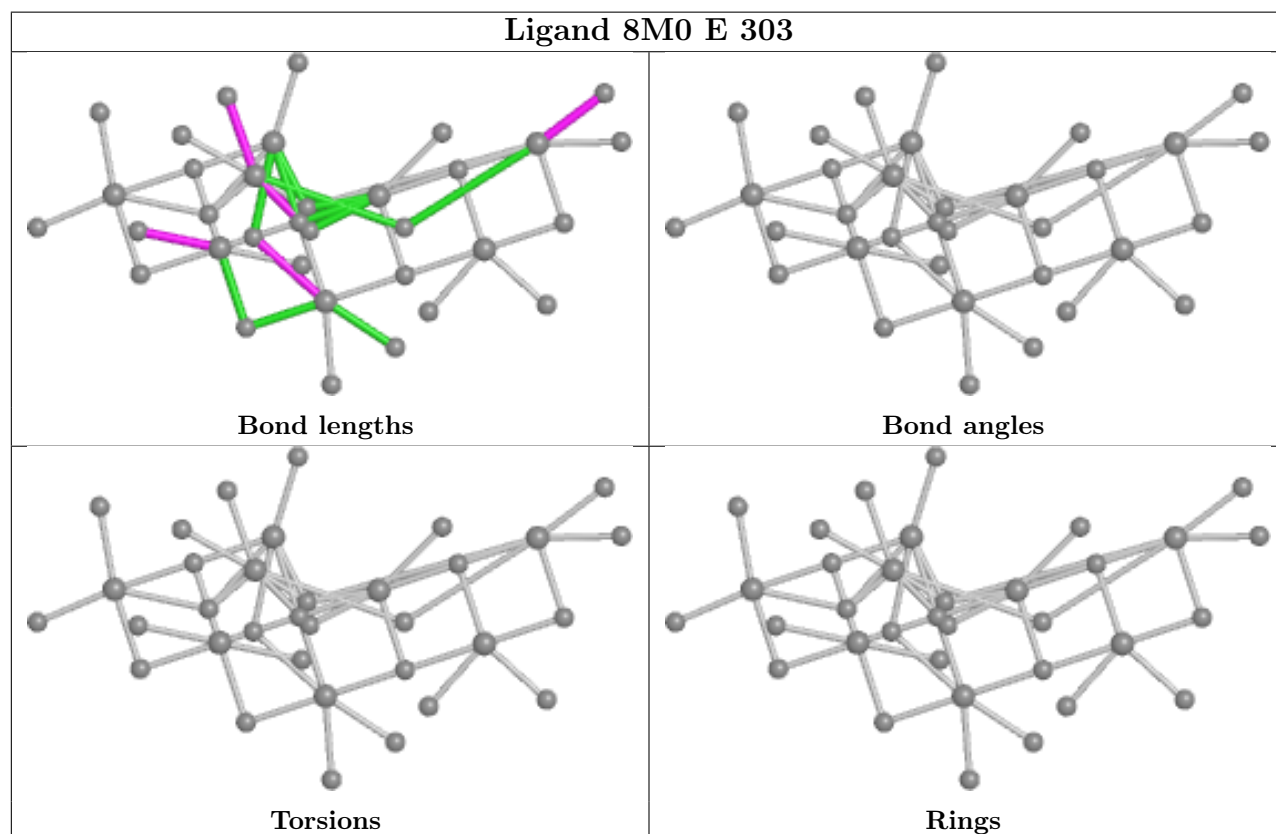
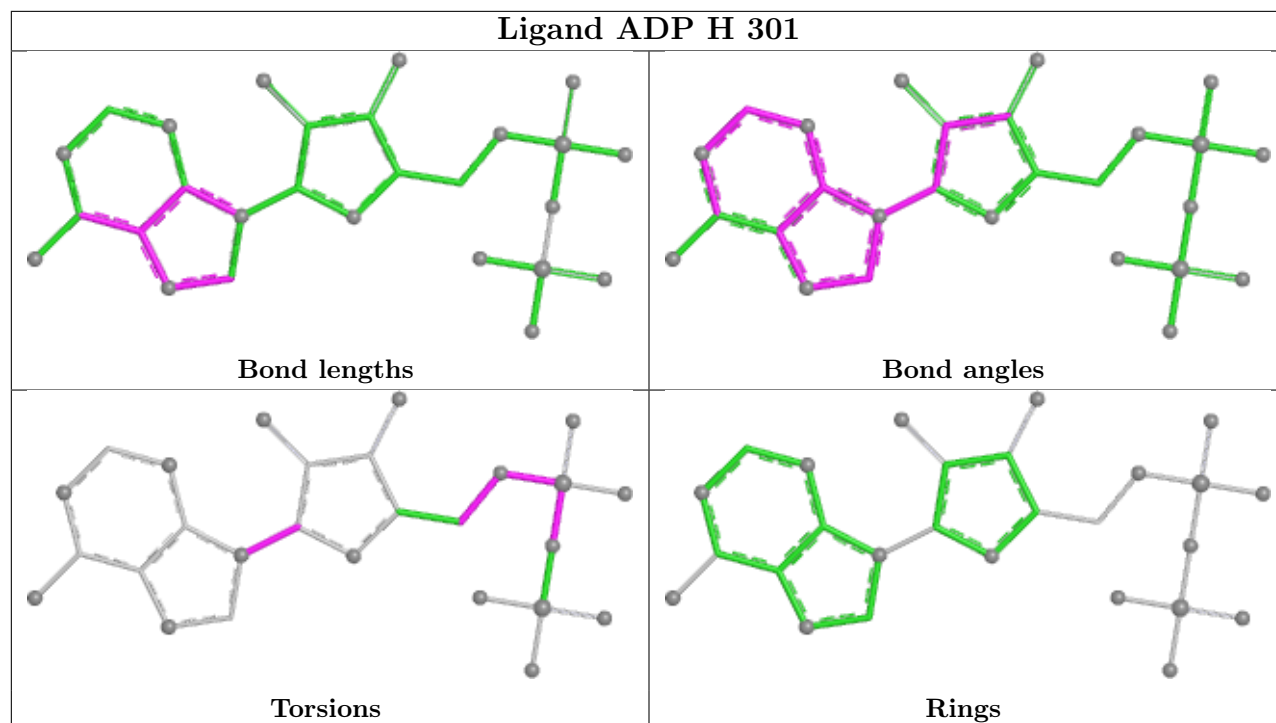


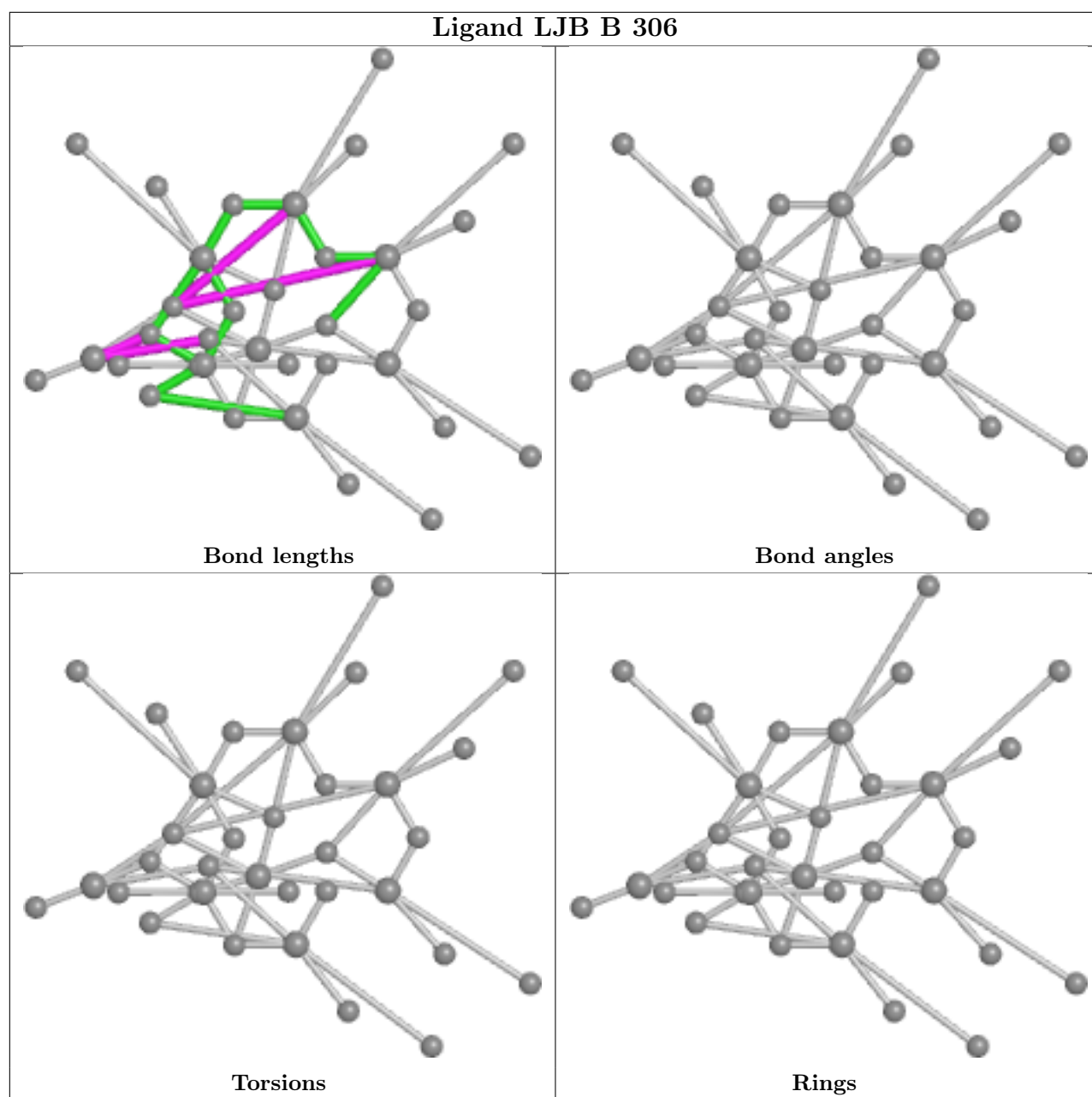
## Ligand ADP F 301

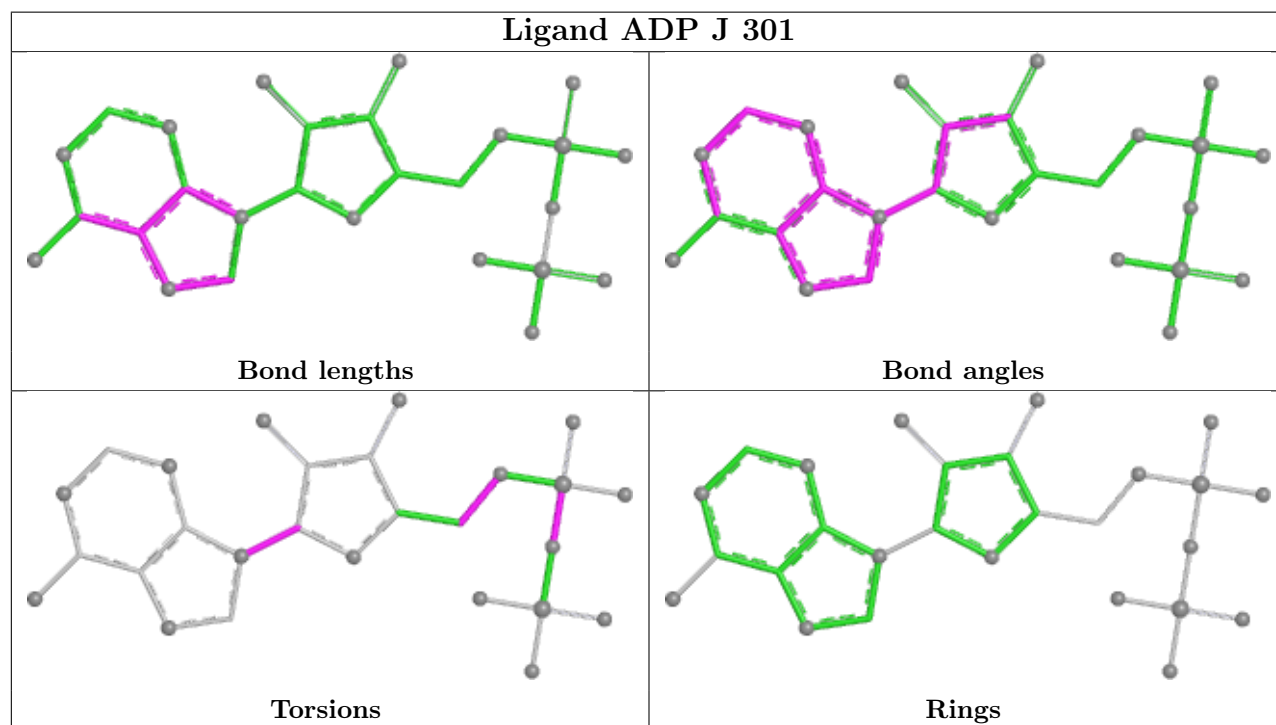
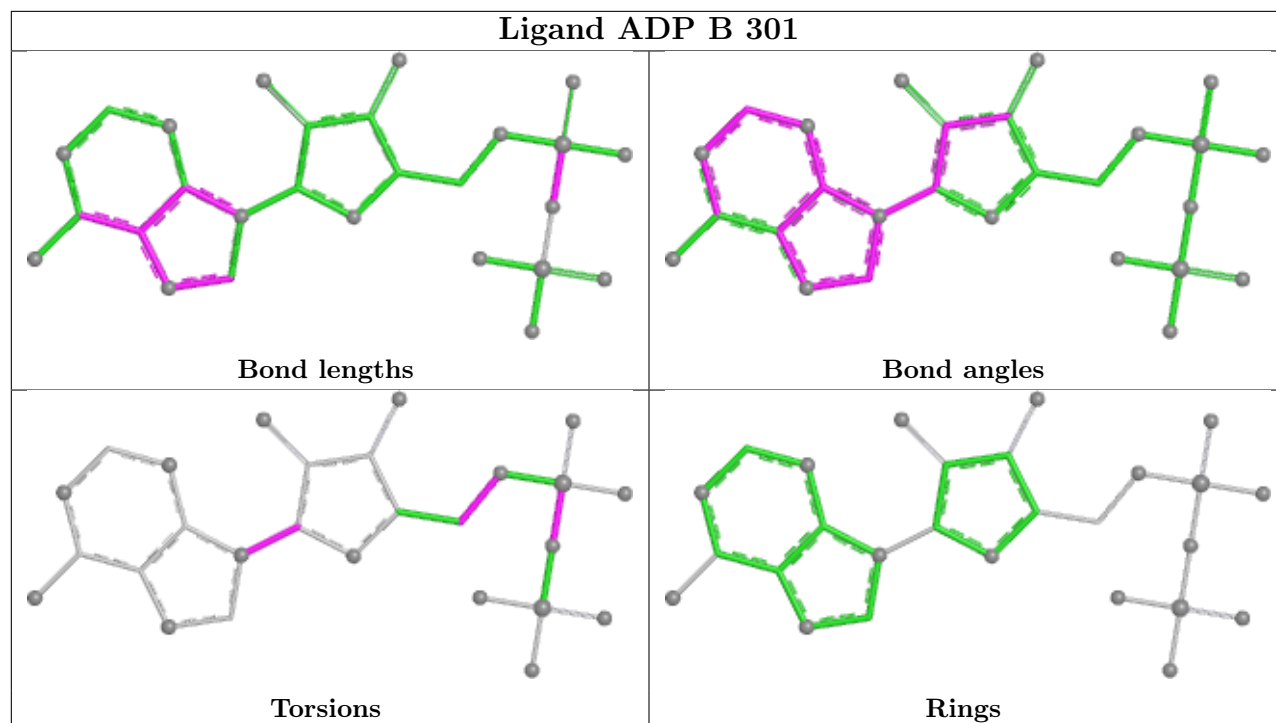


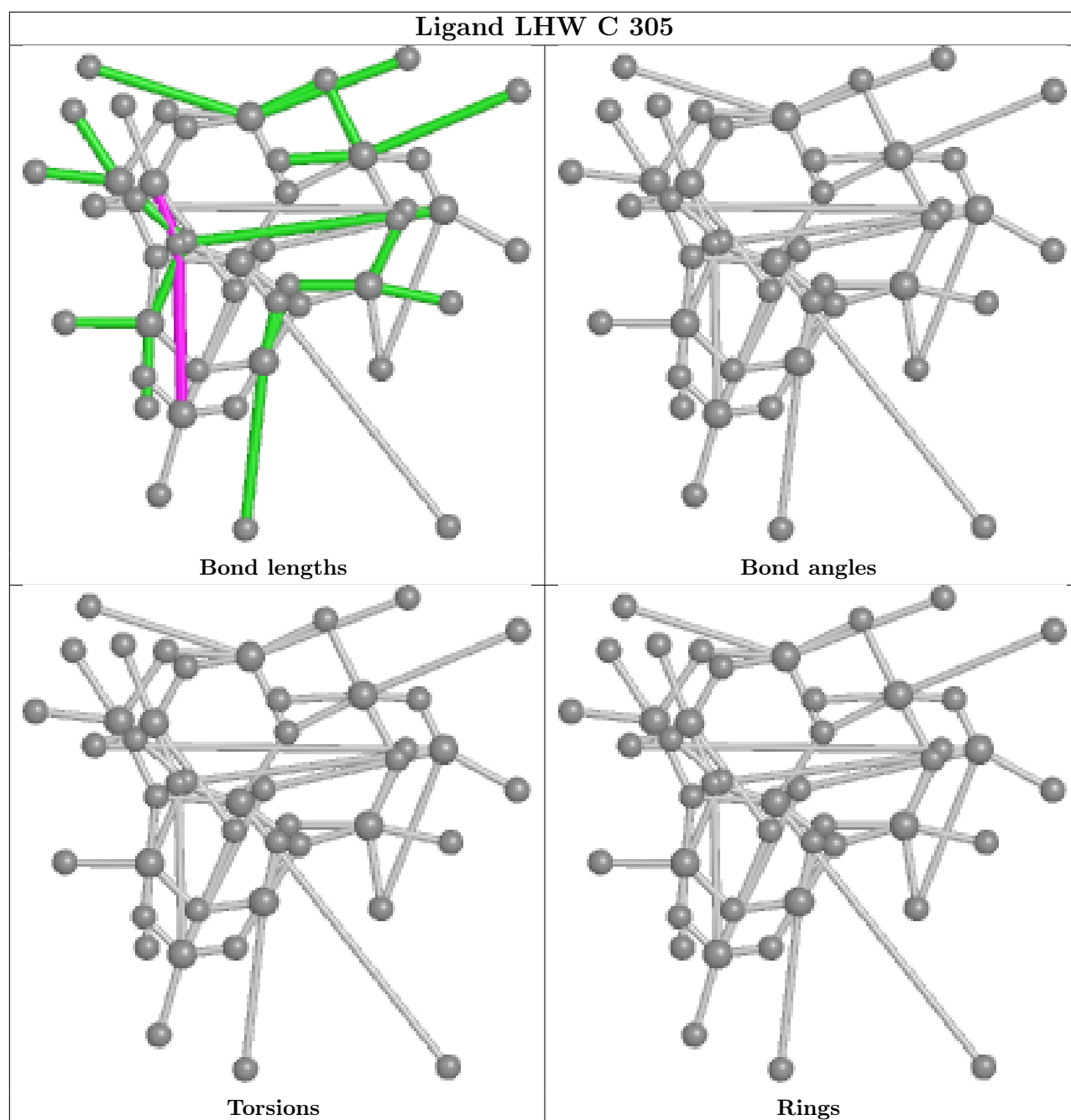












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|-----------------|--------|----------------|-----------------------|---------|
| 1   | B     | 268/269 (99%)   | 0.79   | 27 (10%) 12 13 | 12, 21, 45, 75        | 5 (1%)  |
| 1   | D     | 268/269 (99%)   | 0.91   | 29 (10%) 11 11 | 13, 23, 44, 72        | 4 (1%)  |
| 1   | F     | 269/269 (100%)  | 0.88   | 32 (11%) 9 8   | 11, 24, 49, 85        | 4 (1%)  |
| 1   | H     | 268/269 (99%)   | 1.25   | 40 (14%) 5 5   | 16, 31, 50, 79        | 3 (1%)  |
| 1   | J     | 267/269 (99%)   | 1.05   | 33 (12%) 8 8   | 14, 28, 52, 83        | 6 (2%)  |
| 1   | L     | 267/269 (99%)   | 0.83   | 31 (11%) 9 9   | 15, 24, 45, 66        | 6 (2%)  |
| 2   | A     | 272/275 (98%)   | 0.29   | 16 (5%) 28 31  | 11, 19, 35, 79        | 2 (0%)  |
| 2   | C     | 271/275 (98%)   | 0.41   | 20 (7%) 20 22  | 11, 19, 43, 63        | 2 (0%)  |
| 2   | E     | 272/275 (98%)   | 0.41   | 12 (4%) 39 42  | 12, 21, 43, 65        | 2 (0%)  |
| 2   | G     | 272/275 (98%)   | 0.64   | 20 (7%) 20 22  | 12, 23, 44, 89        | 3 (1%)  |
| 2   | I     | 272/275 (98%)   | 0.78   | 25 (9%) 14 15  | 12, 25, 51, 95        | 2 (0%)  |
| 2   | K     | 272/275 (98%)   | 0.63   | 21 (7%) 19 21  | 13, 22, 49, 74        | 5 (1%)  |
| All | All   | 3238/3264 (99%) | 0.74   | 306 (9%) 14 14 | 11, 23, 48, 95        | 44 (1%) |

All (306) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 130 | GLY  | 17.9 |
| 1   | F     | 131 | LEU  | 17.5 |
| 1   | B     | 129 | ALA  | 15.8 |
| 1   | D     | 130 | GLY  | 15.8 |
| 1   | D     | 129 | ALA  | 14.6 |
| 1   | D     | 128 | GLY  | 13.5 |
| 1   | J     | 131 | LEU  | 13.4 |
| 1   | B     | 128 | GLY  | 13.1 |
| 1   | J     | 130 | GLY  | 12.9 |
| 2   | K     | 5   | THR  | 12.2 |
| 1   | D     | 131 | LEU  | 12.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 131 | LEU  | 12.0 |
| 1   | F     | 130 | GLY  | 11.4 |
| 1   | H     | 129 | ALA  | 11.4 |
| 1   | J     | 129 | ALA  | 11.2 |
| 1   | B     | 131 | LEU  | 11.2 |
| 1   | F     | 129 | ALA  | 10.7 |
| 2   | I     | 276 | ALA  | 10.2 |
| 1   | B     | 127 | GLY  | 9.3  |
| 1   | L     | 129 | ALA  | 8.9  |
| 2   | G     | 275 | PRO  | 8.8  |
| 1   | H     | 128 | GLY  | 8.8  |
| 2   | G     | 276 | ALA  | 8.7  |
| 1   | L     | 128 | GLY  | 8.4  |
| 1   | D     | 127 | GLY  | 8.1  |
| 1   | L     | 131 | LEU  | 7.9  |
| 1   | F     | 128 | GLY  | 7.8  |
| 2   | K     | 275 | PRO  | 7.3  |
| 2   | I     | 275 | PRO  | 7.1  |
| 1   | L     | 4   | SER  | 6.9  |
| 1   | L     | 130 | GLY  | 6.5  |
| 1   | J     | 127 | GLY  | 6.2  |
| 1   | H     | 138 | LEU  | 6.1  |
| 1   | H     | 134 | VAL  | 6.0  |
| 1   | F     | 4   | SER  | 5.9  |
| 2   | A     | 276 | ALA  | 5.8  |
| 2   | K     | 276 | ALA  | 5.8  |
| 1   | H     | 127 | GLY  | 5.8  |
| 2   | A     | 275 | PRO  | 5.8  |
| 2   | G     | 273 | VAL  | 5.6  |
| 1   | F     | 127 | GLY  | 5.5  |
| 1   | J     | 128 | GLY  | 5.5  |
| 2   | G     | 5   | THR  | 5.5  |
| 1   | H     | 130 | GLY  | 5.4  |
| 1   | B     | 134 | VAL  | 5.4  |
| 1   | J     | 4   | SER  | 5.3  |
| 2   | I     | 273 | VAL  | 5.3  |
| 1   | J     | 138 | LEU  | 5.2  |
| 1   | D     | 139 | ALA  | 5.2  |
| 1   | L     | 127 | GLY  | 5.1  |
| 1   | L     | 138 | LEU  | 5.1  |
| 1   | F     | 2   | ALA  | 5.1  |
| 1   | D     | 138 | LEU  | 5.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | K     | 273 | VAL  | 5.0  |
| 1   | F     | 139 | ALA  | 5.0  |
| 1   | F     | 132 | SER  | 4.9  |
| 1   | F     | 138 | LEU  | 4.9  |
| 2   | C     | 6   | ASN  | 4.9  |
| 1   | H     | 139 | ALA  | 4.9  |
| 1   | H     | 4   | SER  | 4.9  |
| 1   | B     | 3   | ASN  | 4.7  |
| 1   | B     | 4   | SER  | 4.7  |
| 1   | J     | 134 | VAL  | 4.6  |
| 1   | L     | 262 | HIS  | 4.6  |
| 2   | I     | 274 | ARG  | 4.6  |
| 2   | K     | 274 | ARG  | 4.6  |
| 1   | H     | 5   | THR  | 4.6  |
| 2   | C     | 272 | GLY  | 4.6  |
| 1   | F     | 137 | SER  | 4.6  |
| 1   | B     | 5   | THR  | 4.5  |
| 1   | B     | 132 | SER  | 4.5  |
| 1   | L     | 139 | ALA  | 4.5  |
| 2   | A     | 274 | ARG  | 4.5  |
| 1   | B     | 135 | PRO  | 4.5  |
| 1   | H     | 222 | HIS  | 4.5  |
| 1   | H     | 141 | VAL  | 4.4  |
| 1   | J     | 139 | ALA  | 4.4  |
| 2   | I     | 5   | THR  | 4.4  |
| 1   | D     | 132 | SER  | 4.4  |
| 1   | B     | 138 | LEU  | 4.4  |
| 1   | J     | 133 | ALA  | 4.3  |
| 1   | F     | 136 | LEU  | 4.3  |
| 1   | J     | 132 | SER  | 4.3  |
| 1   | D     | 3   | ASN  | 4.2  |
| 2   | E     | 5   | THR  | 4.2  |
| 2   | A     | 5   | THR  | 4.2  |
| 2   | G     | 274 | ARG  | 4.2  |
| 1   | H     | 6   | ALA  | 4.1  |
| 1   | J     | 6   | ALA  | 4.1  |
| 2   | I     | 272 | GLY  | 4.1  |
| 1   | B     | 126 | VAL  | 4.1  |
| 1   | F     | 5   | THR  | 4.1  |
| 2   | E     | 276 | ALA  | 4.1  |
| 1   | L     | 263 | VAL  | 4.1  |
| 1   | B     | 6   | ALA  | 4.0  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | F     | 135    | PRO  | 4.0  |
| 1   | H     | 140    | GLU  | 4.0  |
| 1   | D     | 126    | VAL  | 3.8  |
| 2   | K     | 272    | GLY  | 3.8  |
| 1   | H     | 133    | ALA  | 3.8  |
| 1   | D     | 134    | VAL  | 3.8  |
| 1   | J     | 135    | PRO  | 3.8  |
| 1   | F     | 6      | ALA  | 3.8  |
| 1   | D     | 5      | THR  | 3.8  |
| 2   | E     | 224    | GLY  | 3.7  |
| 2   | I     | 6      | ASN  | 3.7  |
| 2   | I     | 203    | PRO  | 3.7  |
| 1   | L     | 5      | THR  | 3.7  |
| 2   | K     | 31     | GLY  | 3.7  |
| 1   | B     | 137[A] | SER  | 3.7  |
| 1   | H     | 3      | ASN  | 3.7  |
| 1   | H     | 135    | PRO  | 3.7  |
| 2   | K     | 222    | SER  | 3.7  |
| 1   | F     | 133    | ALA  | 3.6  |
| 1   | L     | 13     | MET  | 3.6  |
| 1   | B     | 203    | LYS  | 3.5  |
| 1   | F     | 203    | LYS  | 3.5  |
| 1   | J     | 5      | THR  | 3.5  |
| 1   | D     | 4      | SER  | 3.5  |
| 2   | I     | 31     | GLY  | 3.5  |
| 1   | F     | 134    | VAL  | 3.5  |
| 1   | J     | 141    | VAL  | 3.5  |
| 1   | J     | 137    | SER  | 3.5  |
| 2   | I     | 157    | HIS  | 3.5  |
| 1   | B     | 204    | ASP  | 3.5  |
| 1   | D     | 136    | LEU  | 3.5  |
| 1   | L     | 132    | SER  | 3.5  |
| 1   | B     | 139    | ALA  | 3.5  |
| 1   | D     | 137    | SER  | 3.5  |
| 1   | D     | 13     | MET  | 3.5  |
| 2   | A     | 6      | ASN  | 3.4  |
| 1   | D     | 180    | PHE  | 3.4  |
| 1   | H     | 132    | SER  | 3.4  |
| 1   | F     | 3      | ASN  | 3.4  |
| 1   | B     | 180    | PHE  | 3.4  |
| 1   | L     | 137[A] | SER  | 3.4  |
| 1   | F     | 14     | GLN  | 3.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 133 | ALA  | 3.3  |
| 1   | L     | 126 | VAL  | 3.3  |
| 1   | L     | 134 | VAL  | 3.3  |
| 1   | L     | 141 | VAL  | 3.3  |
| 1   | H     | 136 | LEU  | 3.3  |
| 1   | J     | 136 | LEU  | 3.3  |
| 2   | A     | 157 | HIS  | 3.3  |
| 1   | D     | 263 | VAL  | 3.2  |
| 2   | C     | 276 | ALA  | 3.2  |
| 2   | C     | 275 | PRO  | 3.2  |
| 1   | B     | 136 | LEU  | 3.2  |
| 1   | L     | 136 | LEU  | 3.1  |
| 2   | C     | 7   | SER  | 3.1  |
| 1   | L     | 203 | LYS  | 3.1  |
| 1   | F     | 140 | GLU  | 3.1  |
| 1   | J     | 13  | MET  | 3.1  |
| 1   | B     | 141 | VAL  | 3.1  |
| 1   | H     | 176 | LEU  | 3.1  |
| 2   | E     | 6   | ASN  | 3.1  |
| 1   | H     | 206 | THR  | 3.1  |
| 1   | B     | 140 | GLU  | 3.1  |
| 1   | L     | 260 | GLY  | 3.0  |
| 2   | G     | 6   | ASN  | 3.0  |
| 2   | K     | 32  | LYS  | 3.0  |
| 2   | K     | 33  | ARG  | 3.0  |
| 2   | K     | 221 | LYS  | 3.0  |
| 2   | A     | 273 | VAL  | 3.0  |
| 2   | E     | 204 | ASP  | 3.0  |
| 1   | L     | 133 | ALA  | 3.0  |
| 2   | I     | 156 | HIS  | 3.0  |
| 2   | G     | 157 | HIS  | 2.9  |
| 1   | J     | 28  | ALA  | 2.9  |
| 2   | I     | 61  | LEU  | 2.9  |
| 2   | G     | 23  | ARG  | 2.9  |
| 1   | D     | 141 | VAL  | 2.9  |
| 2   | I     | 30  | ALA  | 2.9  |
| 1   | D     | 203 | LYS  | 2.9  |
| 2   | G     | 33  | ARG  | 2.8  |
| 2   | I     | 208 | ALA  | 2.8  |
| 2   | C     | 31  | GLY  | 2.8  |
| 1   | H     | 124 | PRO  | 2.8  |
| 1   | J     | 176 | LEU  | 2.8  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | F     | 13     | MET  | 2.8  |
| 1   | B     | 133    | ALA  | 2.8  |
| 1   | D     | 6      | ALA  | 2.8  |
| 1   | H     | 137[A] | SER  | 2.8  |
| 1   | H     | 125    | VAL  | 2.8  |
| 1   | J     | 140    | GLU  | 2.8  |
| 2   | G     | 272    | GLY  | 2.8  |
| 2   | K     | 207    | GLN  | 2.7  |
| 2   | K     | 30     | ALA  | 2.7  |
| 1   | F     | 180    | PHE  | 2.7  |
| 1   | J     | 204    | ASP  | 2.7  |
| 2   | A     | 156    | HIS  | 2.7  |
| 2   | I     | 32     | LYS  | 2.7  |
| 1   | H     | 7      | GLU  | 2.7  |
| 1   | D     | 202    | SER  | 2.7  |
| 1   | F     | 141    | VAL  | 2.6  |
| 2   | K     | 205    | ARG  | 2.6  |
| 1   | L     | 135    | PRO  | 2.6  |
| 1   | H     | 180    | PHE  | 2.6  |
| 2   | C     | 23     | ARG  | 2.6  |
| 1   | J     | 7      | GLU  | 2.6  |
| 2   | C     | 157    | HIS  | 2.6  |
| 1   | D     | 206    | THR  | 2.6  |
| 2   | E     | 207    | GLN  | 2.6  |
| 1   | D     | 176    | LEU  | 2.6  |
| 1   | F     | 176    | LEU  | 2.6  |
| 1   | J     | 203    | LYS  | 2.6  |
| 2   | K     | 12     | ILE  | 2.6  |
| 2   | C     | 30     | ALA  | 2.6  |
| 1   | F     | 7      | GLU  | 2.6  |
| 1   | B     | 176    | LEU  | 2.5  |
| 1   | J     | 22     | LEU  | 2.5  |
| 1   | L     | 270    | SER  | 2.5  |
| 1   | L     | 125    | VAL  | 2.5  |
| 2   | C     | 8      | ILE  | 2.5  |
| 1   | J     | 218    | ALA  | 2.5  |
| 2   | C     | 32     | LYS  | 2.5  |
| 2   | G     | 67     | LYS  | 2.5  |
| 1   | D     | 204    | ASP  | 2.5  |
| 2   | I     | 11     | VAL  | 2.5  |
| 2   | I     | 12     | ILE  | 2.5  |
| 1   | H     | 219    | LYS  | 2.5  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | B     | 13    | MET  | 2.5  |
| 1   | J     | 14[A] | GLN  | 2.5  |
| 1   | J     | 180   | PHE  | 2.5  |
| 1   | L     | 204   | ASP  | 2.5  |
| 2   | I     | 200   | PRO  | 2.5  |
| 2   | E     | 157   | HIS  | 2.5  |
| 2   | I     | 224   | GLY  | 2.5  |
| 1   | H     | 202   | SER  | 2.5  |
| 2   | E     | 275   | PRO  | 2.4  |
| 1   | H     | 263   | VAL  | 2.4  |
| 1   | J     | 123   | ILE  | 2.4  |
| 2   | K     | 6     | ASN  | 2.4  |
| 1   | B     | 101   | GLN  | 2.4  |
| 1   | L     | 116   | GLN  | 2.4  |
| 2   | I     | 207   | GLN  | 2.4  |
| 2   | G     | 224   | GLY  | 2.4  |
| 1   | H     | 142   | ASN  | 2.4  |
| 2   | A     | 220   | ALA  | 2.4  |
| 2   | I     | 217   | THR  | 2.4  |
| 2   | I     | 33    | ARG  | 2.4  |
| 1   | H     | 123   | ILE  | 2.4  |
| 1   | H     | 126   | VAL  | 2.4  |
| 1   | J     | 126   | VAL  | 2.4  |
| 2   | E     | 220   | ALA  | 2.3  |
| 2   | K     | 206   | GLY  | 2.3  |
| 2   | C     | 274   | ARG  | 2.3  |
| 1   | H     | 68    | LYS  | 2.3  |
| 1   | H     | 203   | LYS  | 2.3  |
| 2   | A     | 221   | LYS  | 2.3  |
| 1   | J     | 65    | ALA  | 2.3  |
| 2   | C     | 223   | GLU  | 2.3  |
| 2   | A     | 272   | GLY  | 2.3  |
| 2   | G     | 31    | GLY  | 2.3  |
| 2   | I     | 162   | GLY  | 2.3  |
| 1   | F     | 206   | THR  | 2.3  |
| 2   | C     | 222   | SER  | 2.3  |
| 2   | C     | 221   | LYS  | 2.3  |
| 2   | C     | 28    | PRO  | 2.2  |
| 1   | F     | 256   | ARG  | 2.2  |
| 1   | H     | 13    | MET  | 2.2  |
| 2   | K     | 156   | HIS  | 2.2  |
| 2   | C     | 273   | VAL  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | G     | 206 | GLY  | 2.2  |
| 2   | C     | 270 | ARG  | 2.2  |
| 2   | K     | 35  | ILE  | 2.2  |
| 1   | J     | 124 | PRO  | 2.2  |
| 1   | L     | 259 | ALA  | 2.2  |
| 1   | F     | 11  | LEU  | 2.2  |
| 2   | C     | 209 | ARG  | 2.2  |
| 2   | K     | 157 | HIS  | 2.2  |
| 1   | L     | 180 | PHE  | 2.2  |
| 2   | A     | 217 | THR  | 2.2  |
| 2   | G     | 222 | SER  | 2.2  |
| 2   | A     | 209 | ARG  | 2.1  |
| 2   | G     | 156 | HIS  | 2.1  |
| 2   | A     | 223 | GLU  | 2.1  |
| 1   | H     | 211 | ILE  | 2.1  |
| 2   | G     | 270 | ARG  | 2.1  |
| 1   | F     | 8   | LEU  | 2.1  |
| 1   | H     | 231 | LEU  | 2.1  |
| 1   | H     | 147 | SER  | 2.1  |
| 2   | C     | 207 | GLN  | 2.1  |
| 2   | I     | 222 | SER  | 2.1  |
| 2   | E     | 205 | ARG  | 2.1  |
| 1   | F     | 28  | ALA  | 2.1  |
| 1   | H     | 54  | ALA  | 2.1  |
| 1   | J     | 205 | ALA  | 2.1  |
| 2   | A     | 30  | ALA  | 2.1  |
| 1   | F     | 125 | VAL  | 2.1  |
| 2   | I     | 223 | GLU  | 2.1  |
| 2   | E     | 222 | SER  | 2.1  |
| 1   | D     | 11  | LEU  | 2.1  |
| 2   | G     | 25  | LEU  | 2.1  |
| 1   | L     | 123 | ILE  | 2.1  |
| 1   | L     | 6   | ALA  | 2.0  |
| 2   | G     | 30  | ALA  | 2.0  |
| 2   | K     | 220 | ALA  | 2.0  |
| 1   | D     | 125 | VAL  | 2.0  |
| 1   | H     | 270 | SER  | 2.0  |
| 2   | A     | 7   | SER  | 2.0  |
| 1   | D     | 262 | HIS  | 2.0  |
| 2   | E     | 223 | GLU  | 2.0  |
| 1   | L     | 256 | ARG  | 2.0  |
| 2   | G     | 27  | ARG  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 68  | LYS  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|----------------------------|-------|
| 5   | 8M0  | J     | 302    | 36/36 | 0.77 | 0.30 | 72,77,81,82                | 36    |
| 7   | PO4  | L     | 305[B] | 5/5   | 0.81 | 0.16 | 20,20,22,25                | 5     |
| 5   | 8M0  | H     | 303    | 36/36 | 0.82 | 0.27 | 56,61,66,67                | 36    |
| 5   | 8M0  | L     | 303    | 36/36 | 0.88 | 0.21 | 41,44,50,52                | 36    |
| 5   | 8M0  | F     | 303    | 36/36 | 0.89 | 0.20 | 27,37,41,44                | 36    |
| 7   | PO4  | F     | 305[B] | 5/5   | 0.90 | 0.11 | 16,18,20,27                | 5     |
| 7   | PO4  | H     | 305[B] | 5/5   | 0.90 | 0.12 | 26,26,28,31                | 5     |
| 7   | PO4  | J     | 305[B] | 5/5   | 0.90 | 0.14 | 22,26,29,30                | 5     |
| 5   | 8M0  | C     | 301    | 36/36 | 0.90 | 0.20 | 27,36,44,46                | 36    |
| 11  | LHW  | C     | 305    | 45/45 | 0.91 | 0.11 | 40,57,62,63                | 45    |
| 8   | LJB  | B     | 306    | 34/34 | 0.92 | 0.10 | 47,60,63,68                | 34    |
| 8   | LJB  | L     | 306    | 34/34 | 0.92 | 0.10 | 57,64,74,99                | 34    |
| 3   | ADP  | H     | 301    | 27/27 | 0.92 | 0.10 | 25,29,34,35                | 0     |
| 5   | 8M0  | B     | 303    | 36/36 | 0.93 | 0.17 | 25,34,38,39                | 36    |
| 11  | LHW  | K     | 304    | 45/45 | 0.93 | 0.10 | 48,61,66,70                | 44    |
| 3   | ADP  | J     | 301    | 27/27 | 0.94 | 0.08 | 19,25,28,33                | 0     |
| 7   | PO4  | D     | 304[B] | 5/5   | 0.94 | 0.10 | 21,22,24,33                | 5     |
| 3   | ADP  | F     | 301    | 27/27 | 0.95 | 0.08 | 15,20,24,25                | 0     |
| 3   | ADP  | L     | 301    | 27/27 | 0.95 | 0.08 | 18,21,26,29                | 0     |
| 9   | ATP  | G     | 301    | 31/31 | 0.95 | 0.08 | 17,22,27,28                | 0     |
| 9   | ATP  | I     | 301    | 31/31 | 0.95 | 0.09 | 20,26,32,39                | 0     |
| 7   | PO4  | B     | 305[B] | 5/5   | 0.95 | 0.08 | 15,16,18,27                | 5     |

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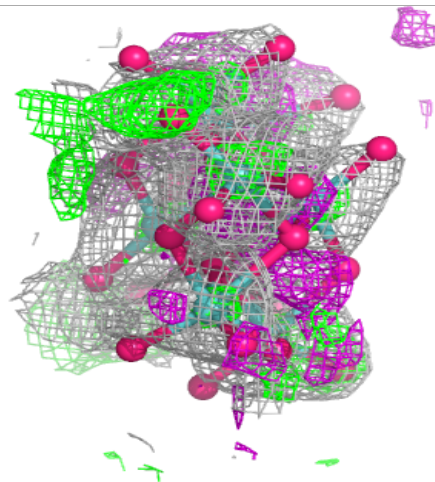
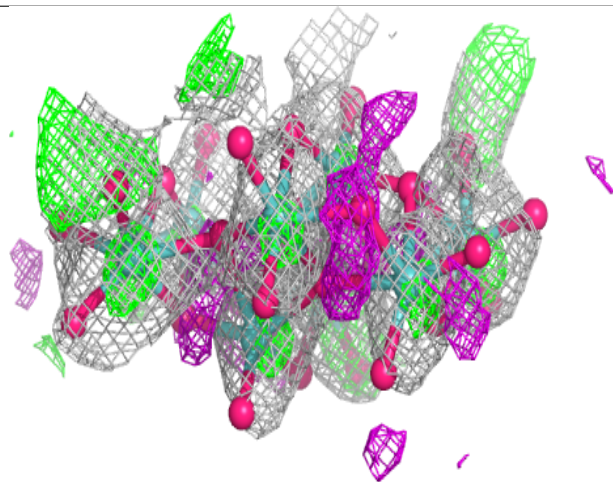
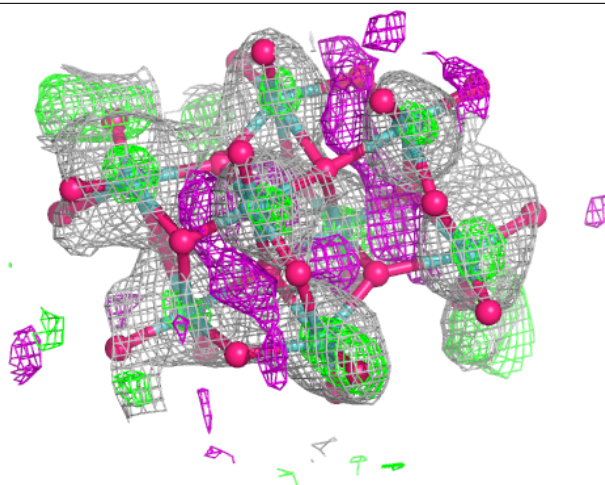
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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 3   | ADP  | D     | 301    | 27/27 | 0.95 | 0.08 | 18,23,28,33                 | 0     |
| 9   | ATP  | K     | 301    | 31/31 | 0.96 | 0.08 | 16,21,26,28                 | 0     |
| 3   | ADP  | B     | 301    | 27/27 | 0.96 | 0.07 | 14,18,21,22                 | 0     |
| 9   | ATP  | C     | 302    | 31/31 | 0.96 | 0.07 | 15,17,23,25                 | 0     |
| 9   | ATP  | E     | 301    | 31/31 | 0.97 | 0.07 | 14,21,25,31                 | 0     |
| 4   | MG   | J     | 303    | 1/1   | 0.97 | 0.14 | 12,12,12,12                 | 1     |
| 4   | MG   | I     | 302    | 1/1   | 0.97 | 0.04 | 19,19,19,19                 | 0     |
| 6   | MOO  | B     | 304[A] | 5/5   | 0.97 | 0.11 | 14,18,23,27                 | 5     |
| 9   | ATP  | A     | 301    | 31/31 | 0.97 | 0.07 | 13,17,19,19                 | 0     |
| 4   | MG   | H     | 302    | 1/1   | 0.97 | 0.06 | 24,24,24,24                 | 0     |
| 5   | 8M0  | K     | 303    | 34/36 | 0.98 | 0.09 | 22,29,34,41                 | 0     |
| 5   | 8M0  | C     | 304    | 34/36 | 0.98 | 0.09 | 18,25,30,37                 | 0     |
| 4   | MG   | D     | 302    | 1/1   | 0.98 | 0.04 | 21,21,21,21                 | 0     |
| 4   | MG   | L     | 302    | 1/1   | 0.98 | 0.07 | 21,21,21,21                 | 0     |
| 4   | MG   | G     | 302    | 1/1   | 0.98 | 0.03 | 19,19,19,19                 | 0     |
| 4   | MG   | C     | 303    | 1/1   | 0.98 | 0.03 | 14,14,14,14                 | 0     |
| 4   | MG   | K     | 302    | 1/1   | 0.99 | 0.03 | 19,19,19,19                 | 0     |
| 5   | 8M0  | G     | 303    | 34/36 | 0.99 | 0.08 | 23,29,35,36                 | 0     |
| 4   | MG   | A     | 302    | 1/1   | 0.99 | 0.04 | 15,15,15,15                 | 0     |
| 5   | 8M0  | I     | 303    | 34/36 | 0.99 | 0.08 | 23,31,37,41                 | 0     |
| 5   | 8M0  | A     | 303    | 34/36 | 0.99 | 0.08 | 15,26,31,40                 | 0     |
| 4   | MG   | F     | 302    | 1/1   | 0.99 | 0.05 | 17,17,17,17                 | 0     |
| 4   | MG   | E     | 302    | 1/1   | 0.99 | 0.03 | 19,19,19,19                 | 0     |
| 6   | MOO  | D     | 303[A] | 5/5   | 0.99 | 0.07 | 17,19,23,24                 | 5     |
| 6   | MOO  | F     | 304[A] | 5/5   | 0.99 | 0.06 | 14,18,20,20                 | 5     |
| 6   | MOO  | H     | 304[A] | 5/5   | 0.99 | 0.09 | 25,27,30,31                 | 5     |
| 6   | MOO  | J     | 304[A] | 5/5   | 0.99 | 0.11 | 21,24,25,29                 | 5     |
| 6   | MOO  | L     | 304[A] | 5/5   | 0.99 | 0.07 | 18,19,22,22                 | 5     |
| 10  | M10  | G     | 304    | 13/16 | 0.99 | 0.06 | 16,22,24,27                 | 0     |
| 4   | MG   | B     | 302    | 1/1   | 0.99 | 0.02 | 16,16,16,16                 | 0     |
| 5   | 8M0  | E     | 303    | 34/36 | 0.99 | 0.08 | 18,26,30,37                 | 0     |
| 10  | M10  | A     | 304    | 13/16 | 1.00 | 0.04 | 16,18,23,23                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

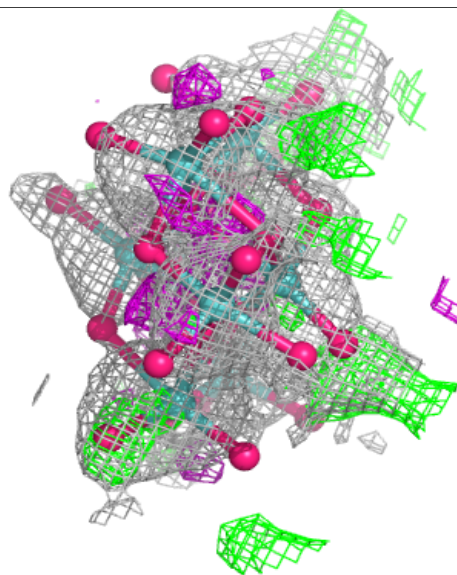
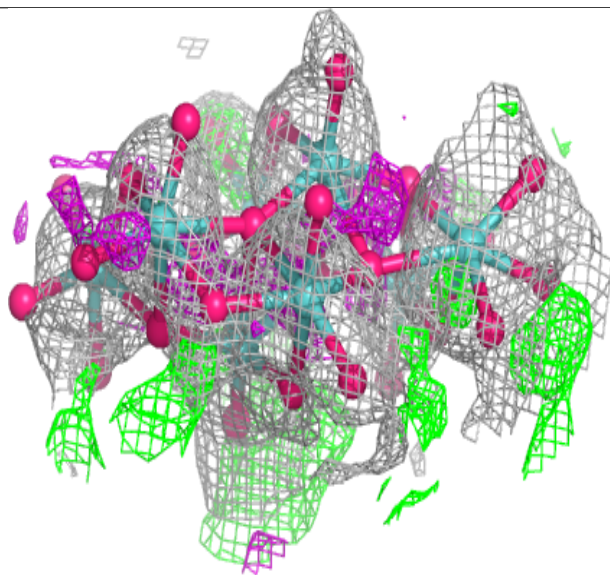
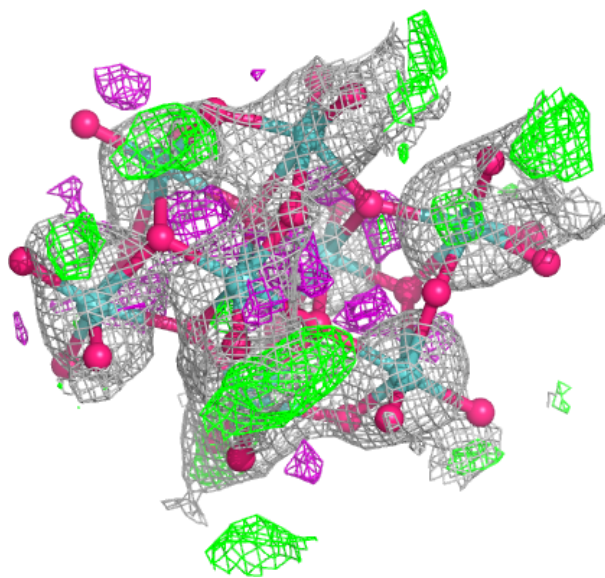
**Electron density around 8M0 J 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



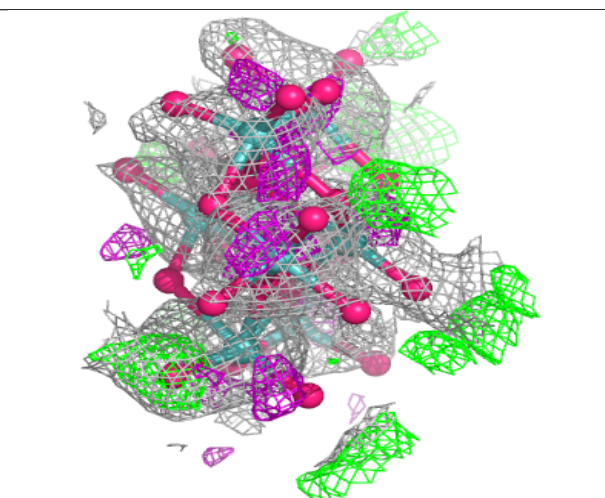
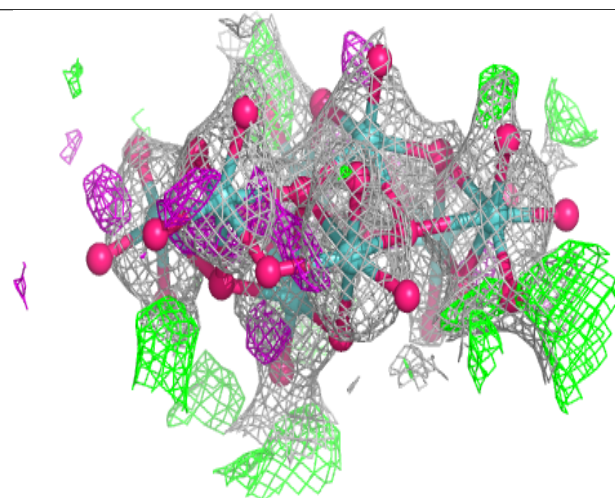
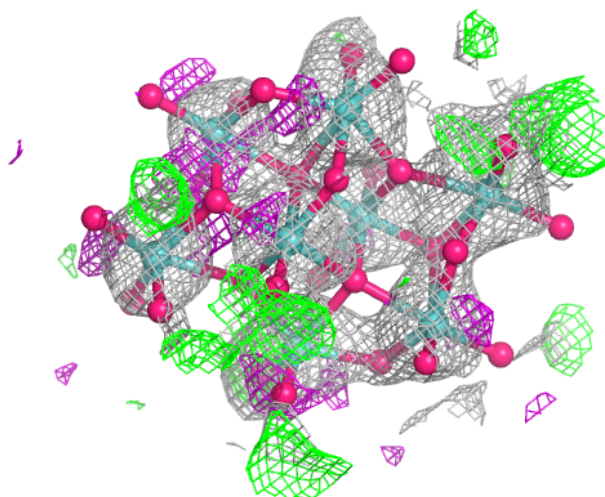
**Electron density around 8M0 H 303:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



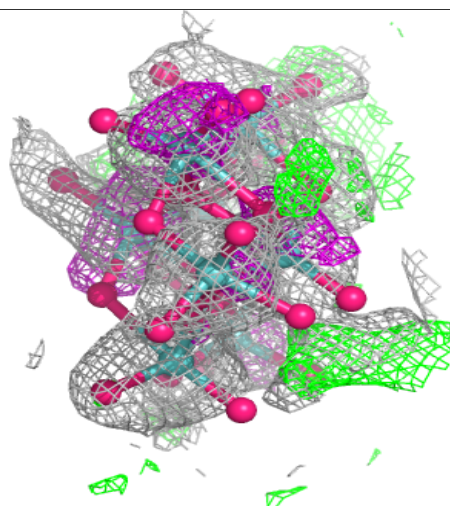
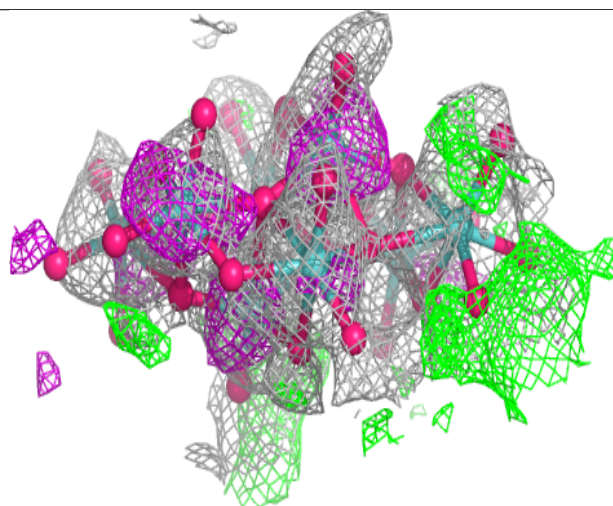
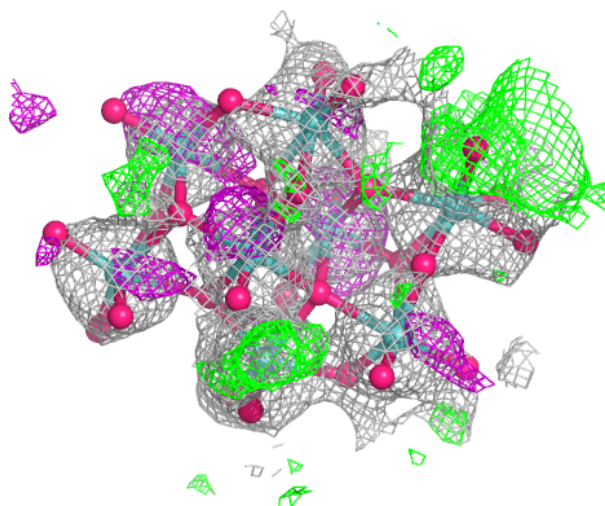
**Electron density around 8M0 L 303:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



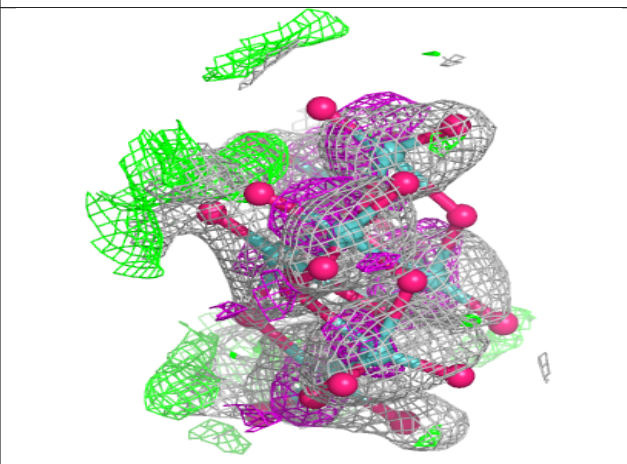
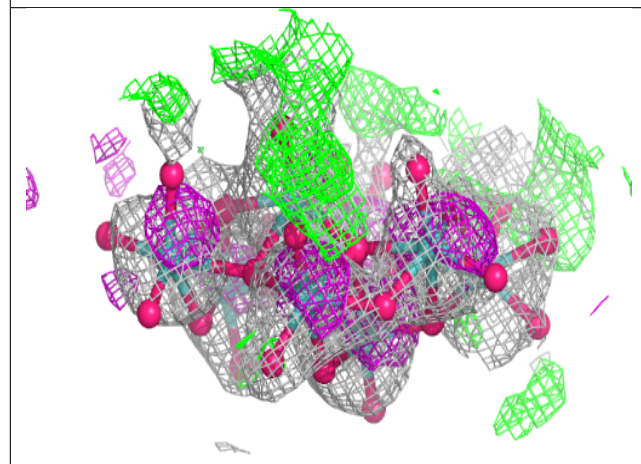
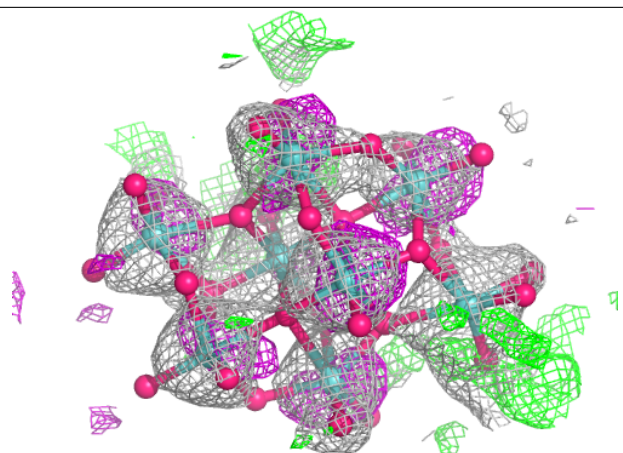
**Electron density around 8M0 F 303:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



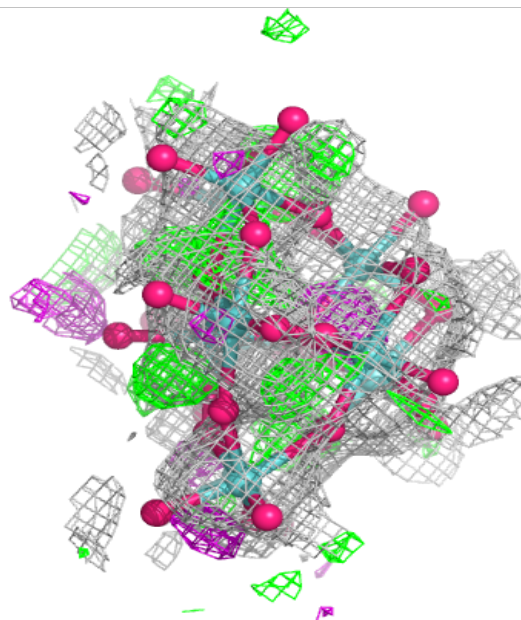
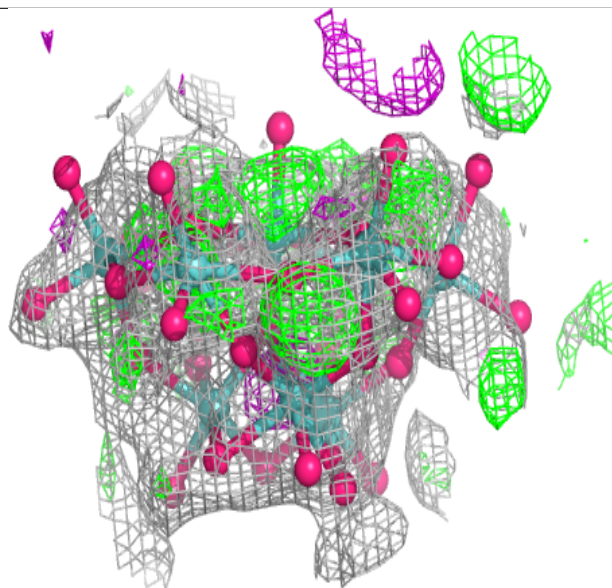
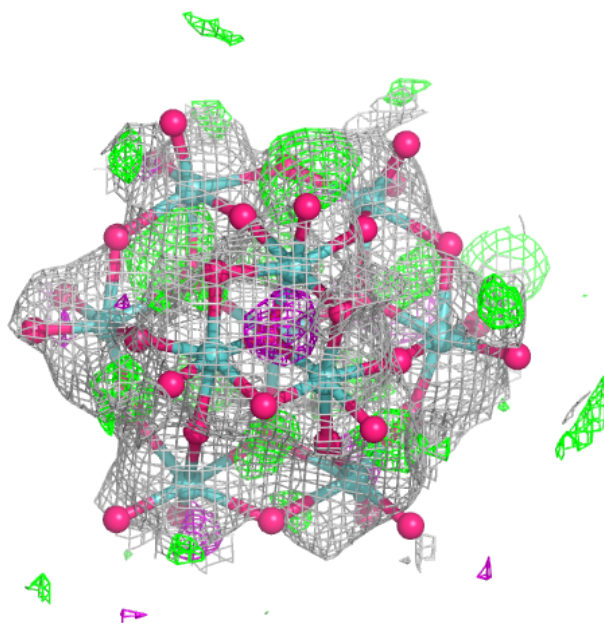
**Electron density around 8M0 C 301:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



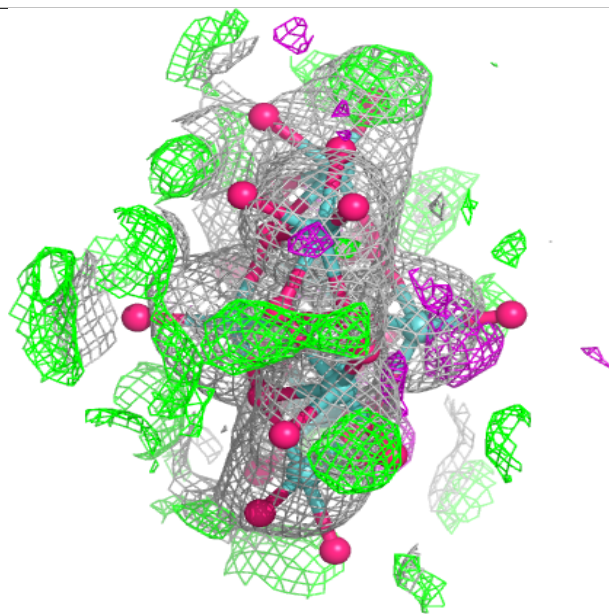
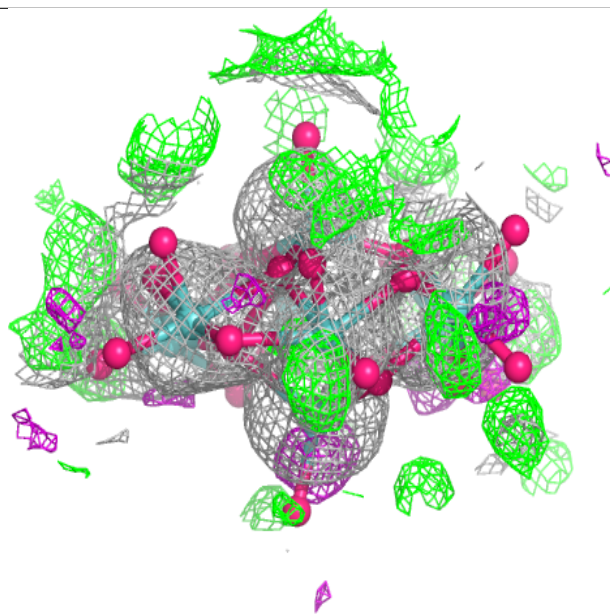
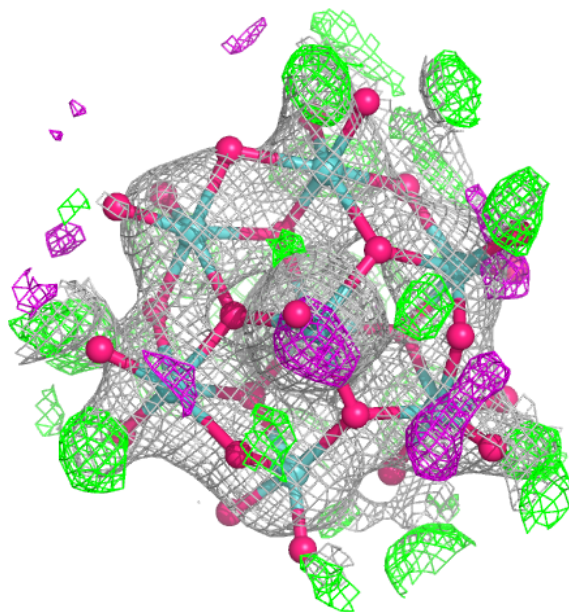
**Electron density around LHW C 305:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



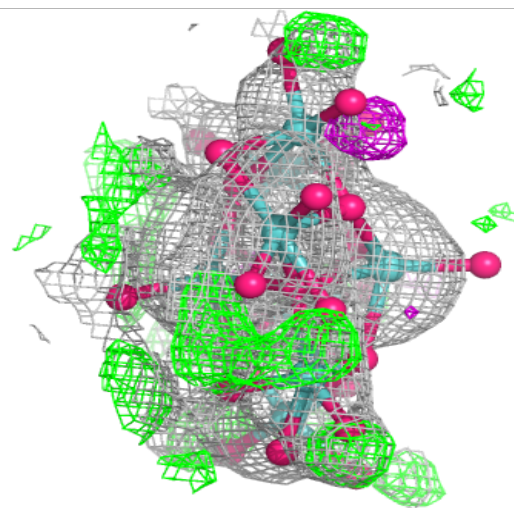
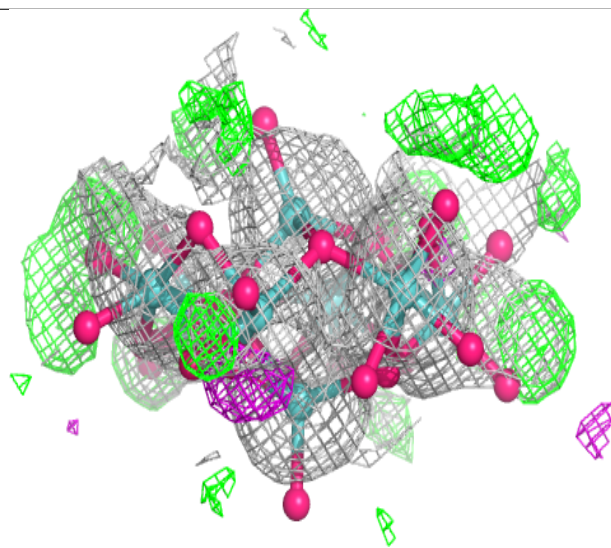
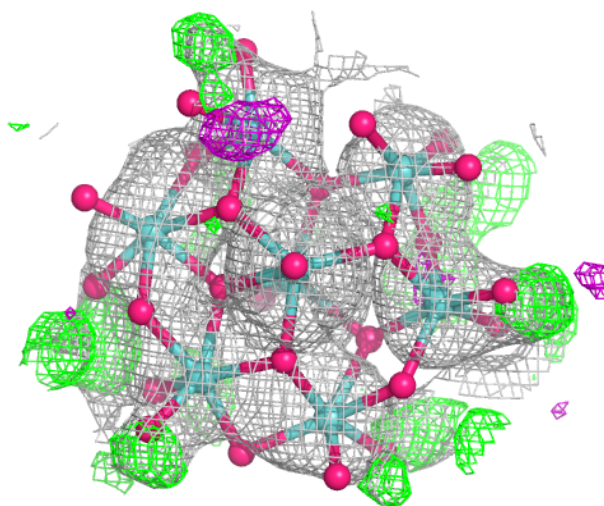
**Electron density around LJB B 306:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



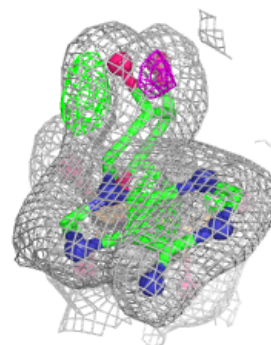
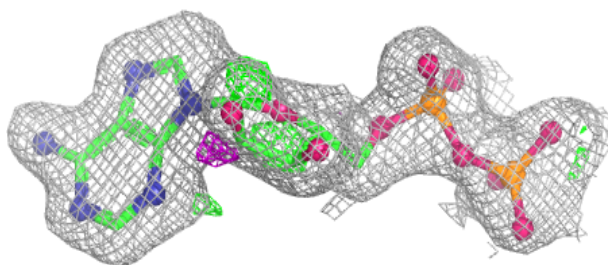
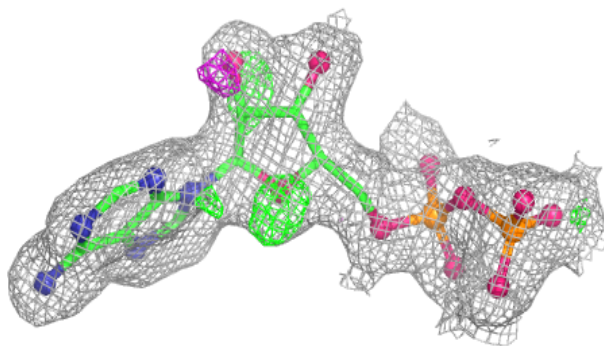
**Electron density around LJB L 306:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

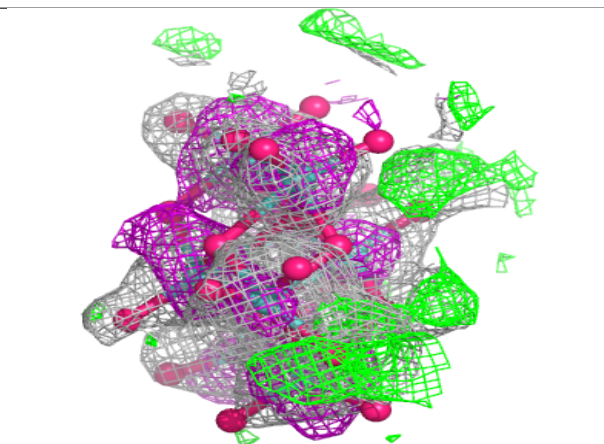
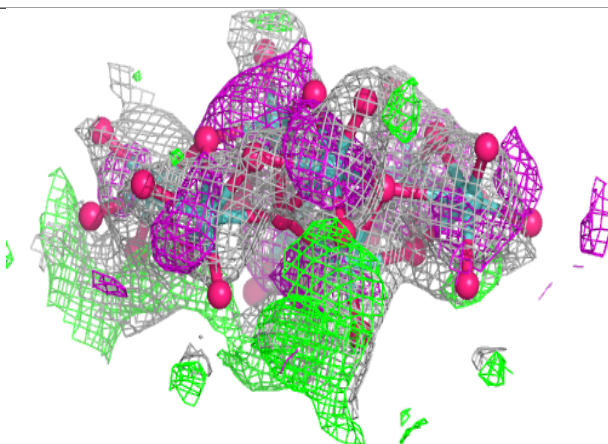
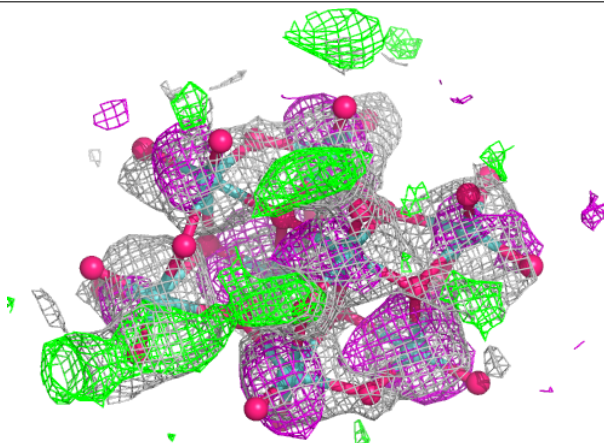


**Electron density around ADP H 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

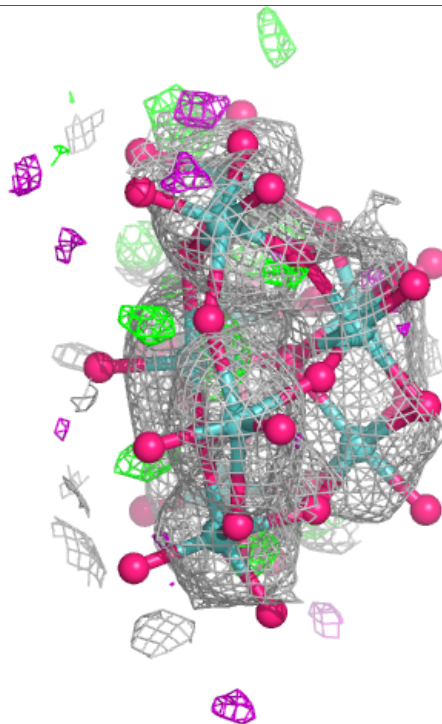
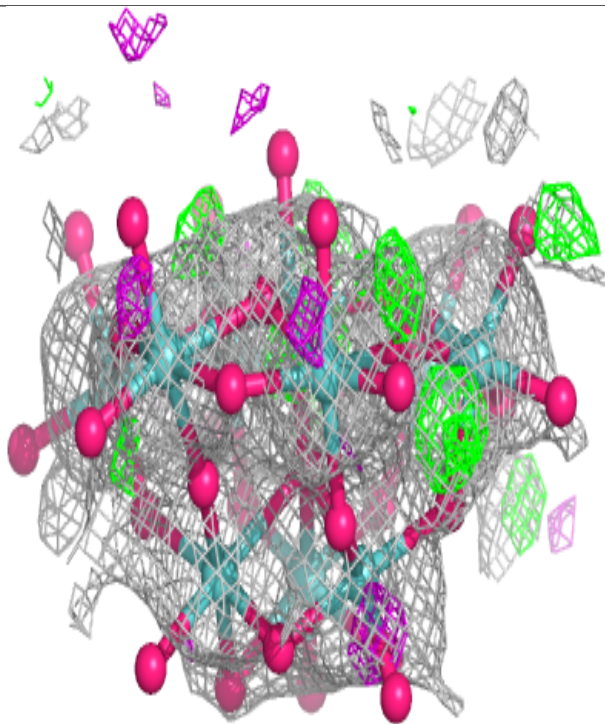
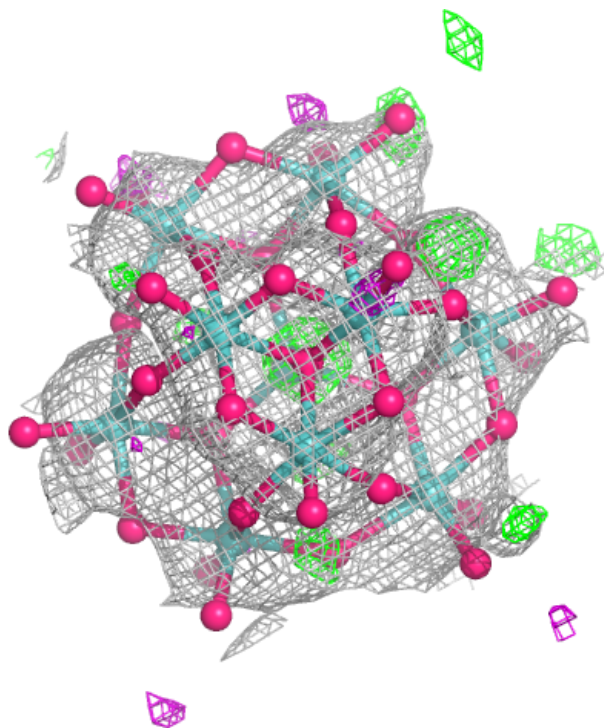
**Electron density around 8M0 B 303:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



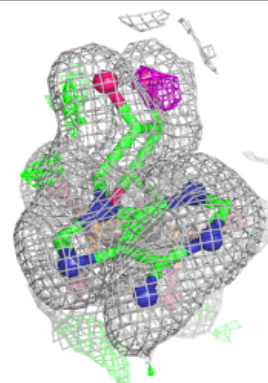
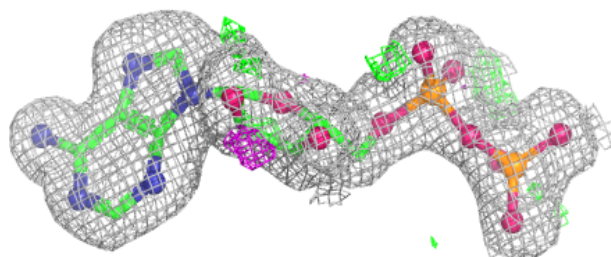
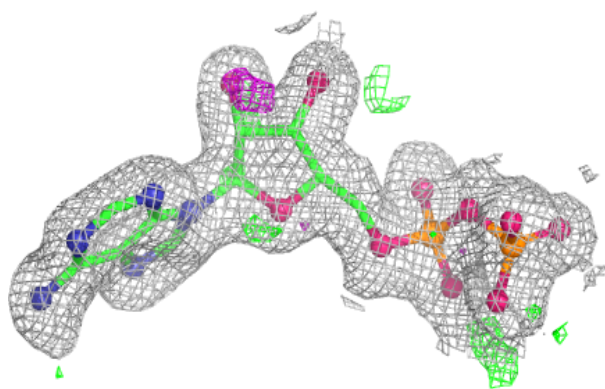
**Electron density around LHW K 304:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

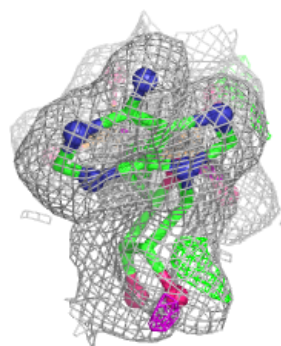
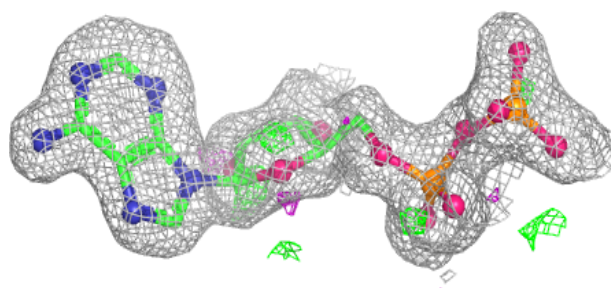
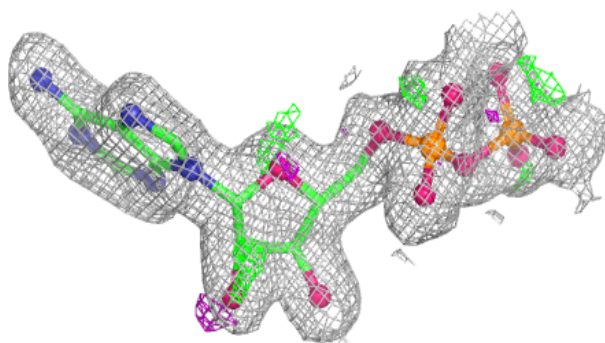


**Electron density around ADP J 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

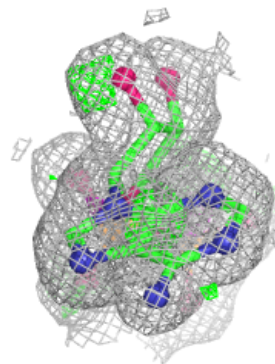
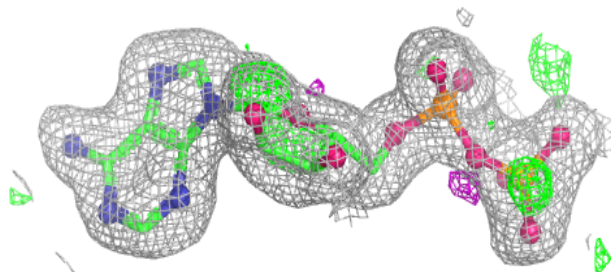
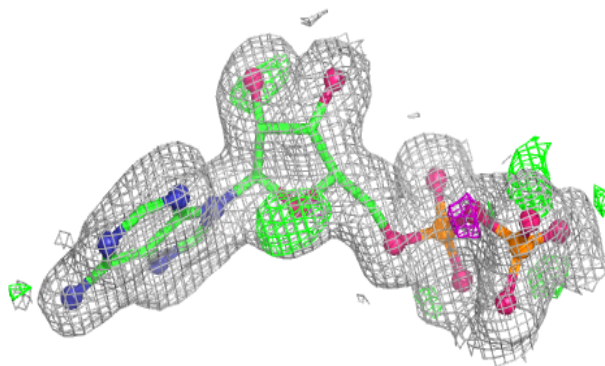
**Electron density around ADP F 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

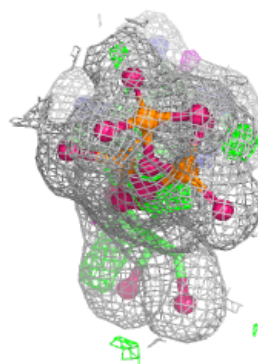
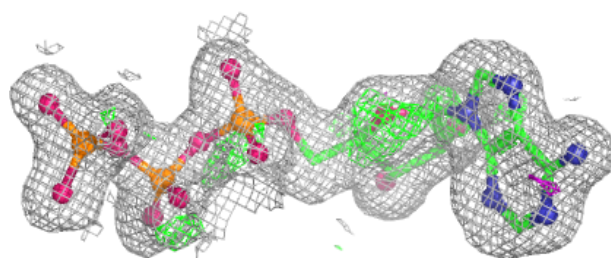
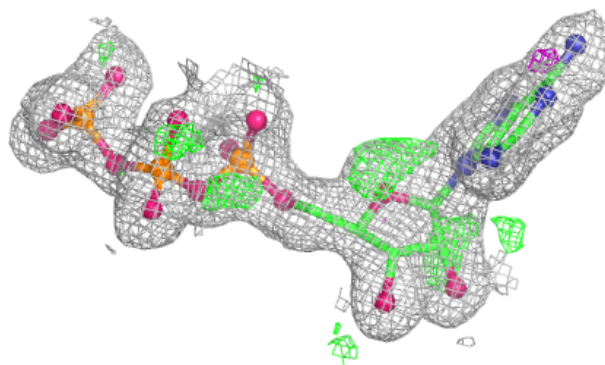


**Electron density around ADP L 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

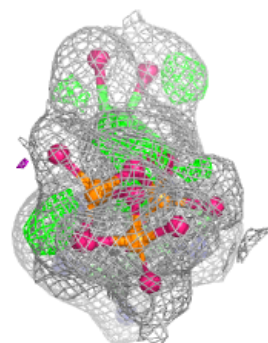
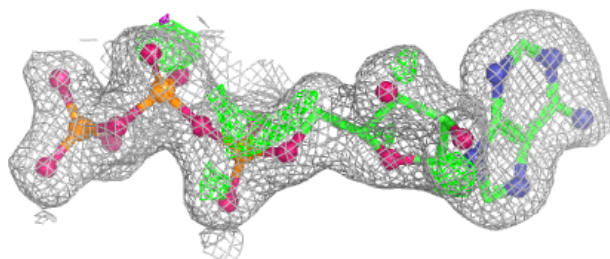
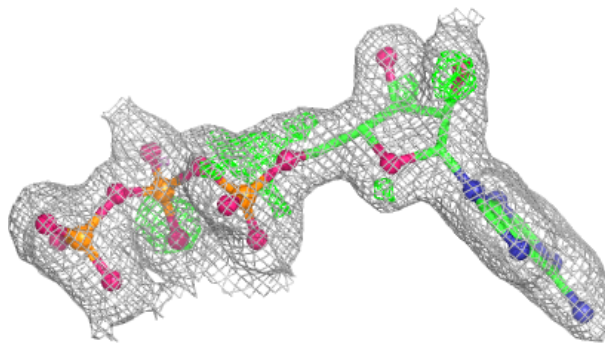
**Electron density around ATP G 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

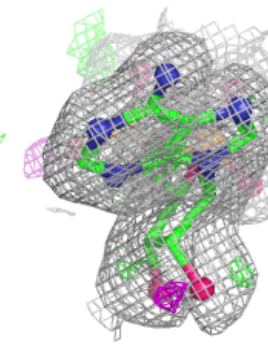
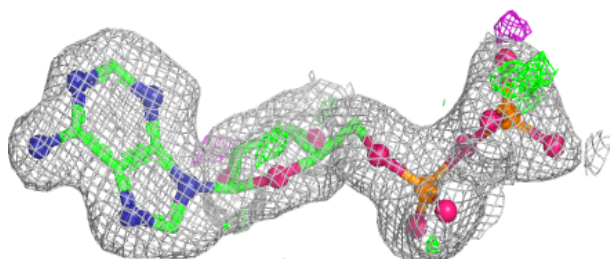
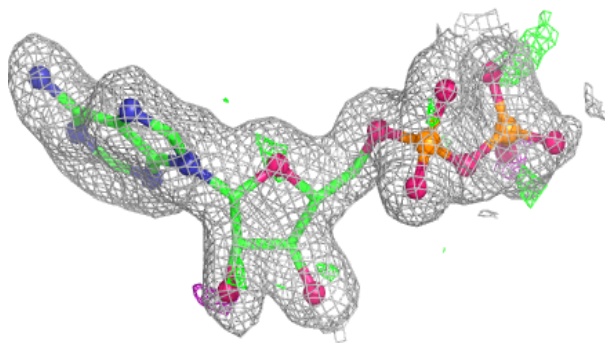


**Electron density around ATP I 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

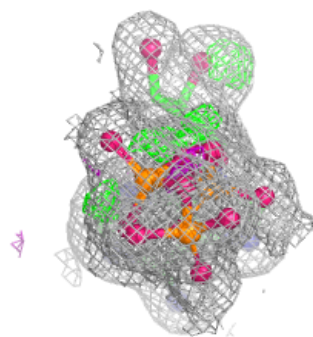
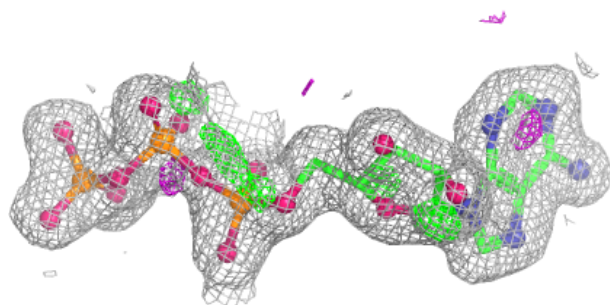
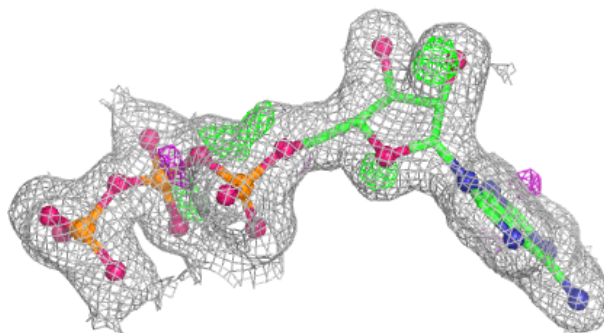
**Electron density around ADP D 301:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

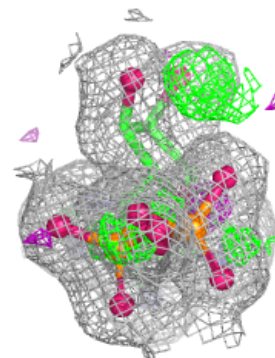
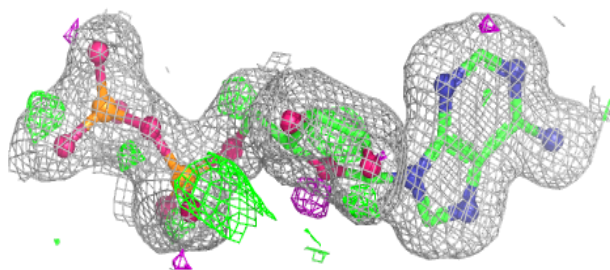
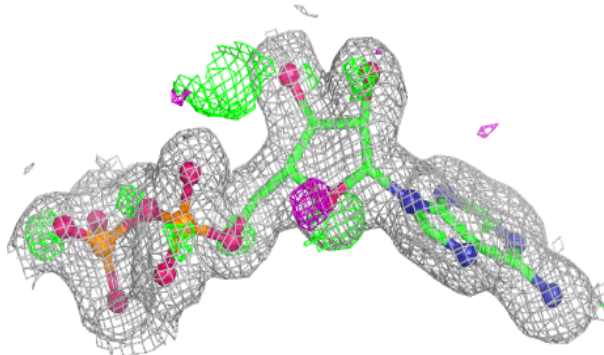


**Electron density around ATP K 301:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

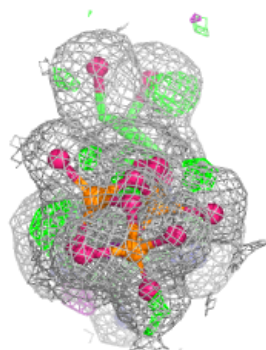
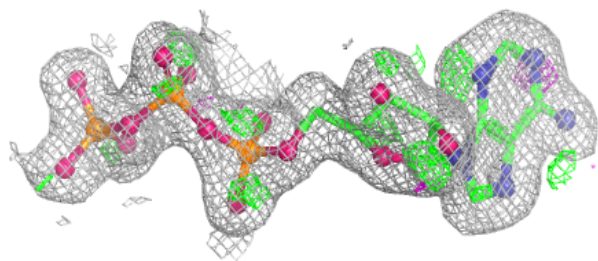
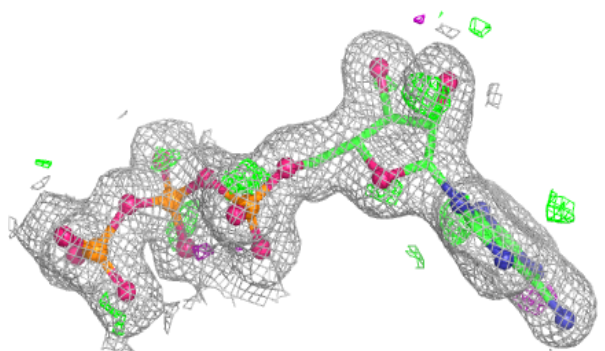
**Electron density around ADP B 301:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

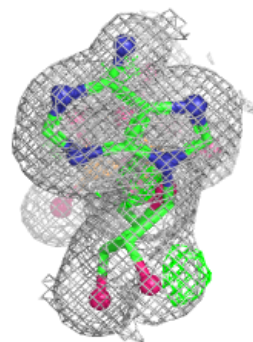
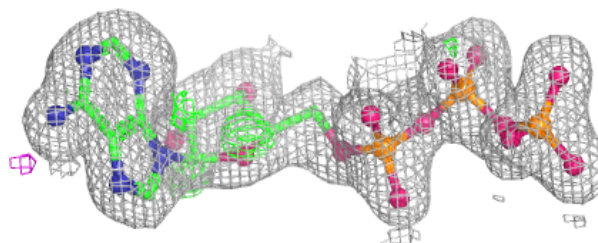
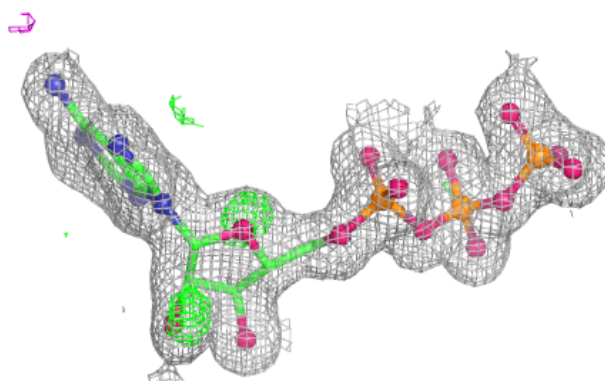


**Electron density around ATP C 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

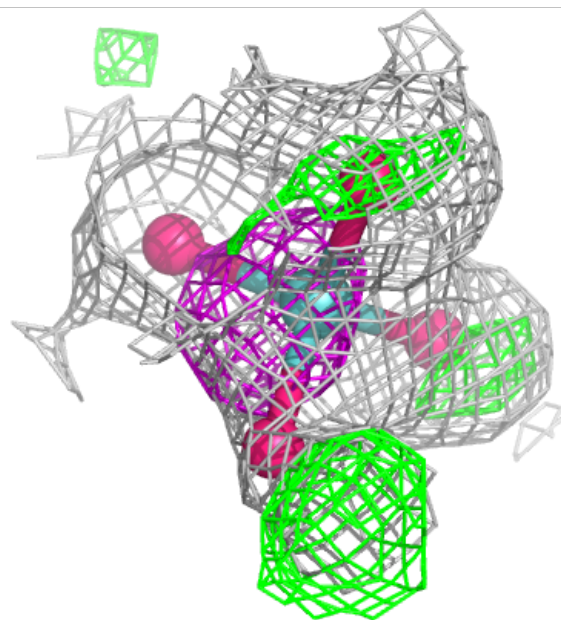
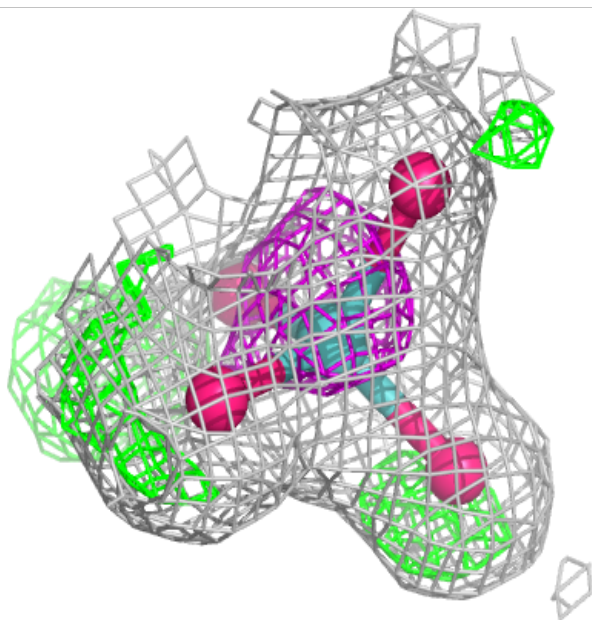
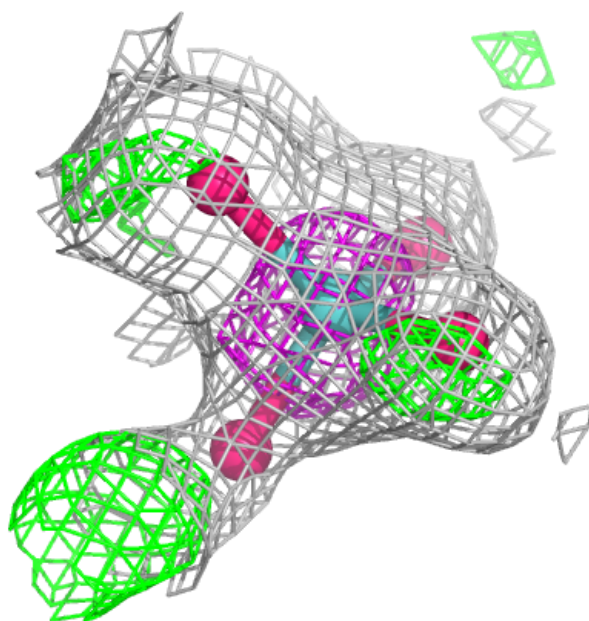
**Electron density around ATP E 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



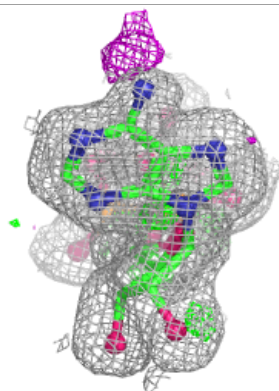
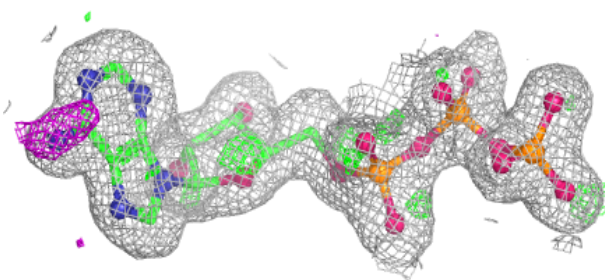
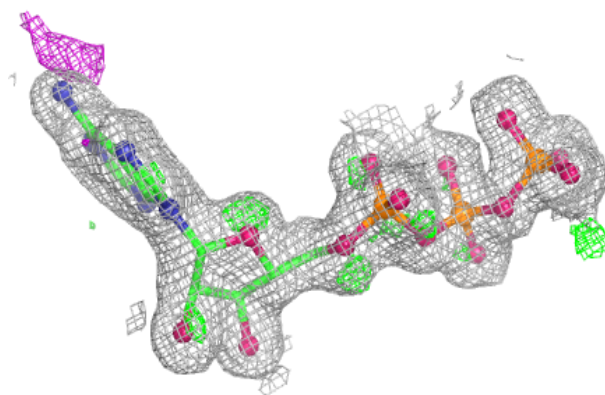
**Electron density around MOO B 304 (A):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



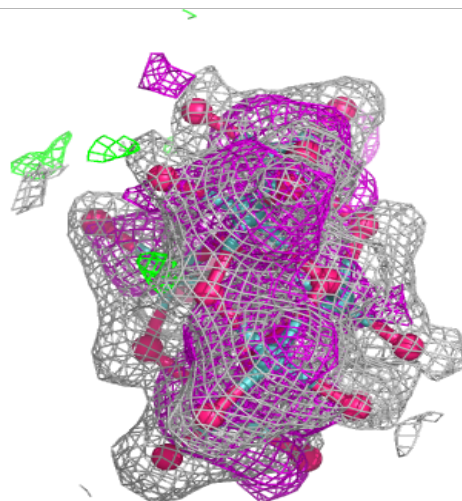
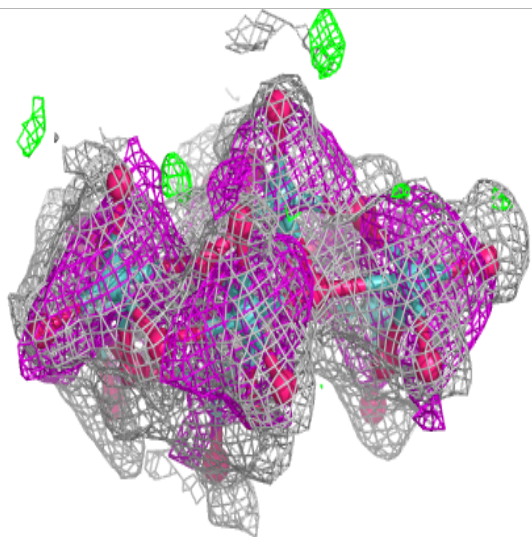
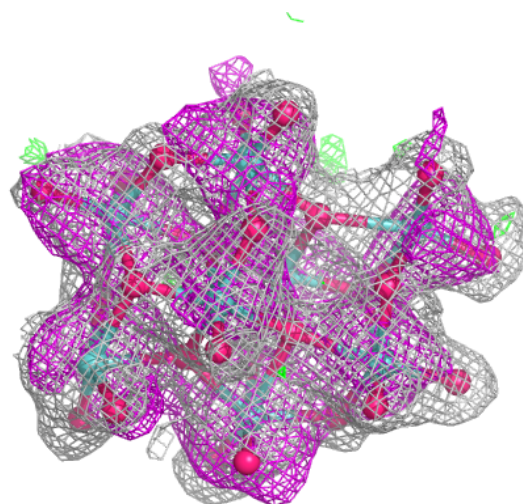
**Electron density around ATP A 301:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



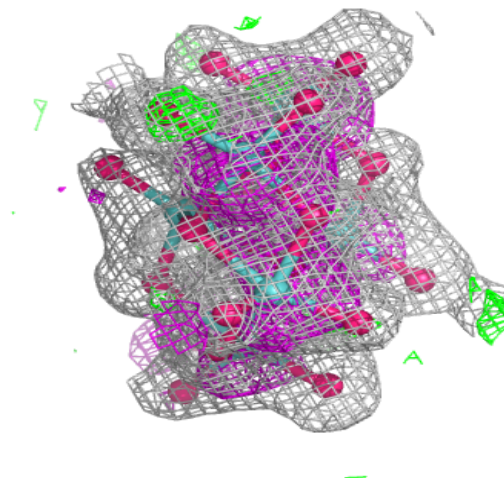
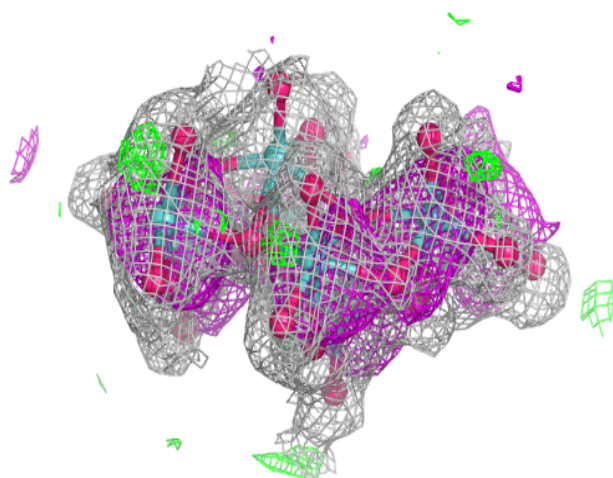
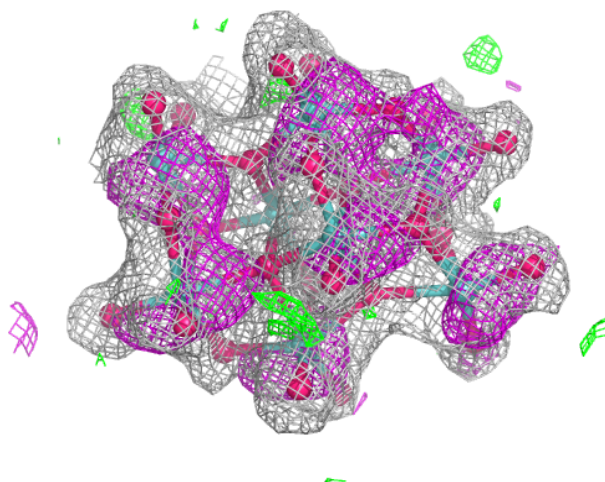
**Electron density around 8M0 K 303:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



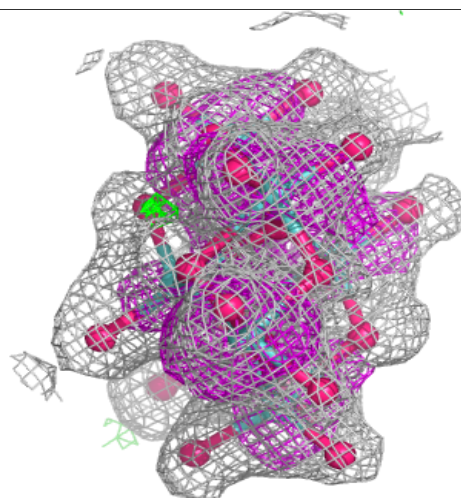
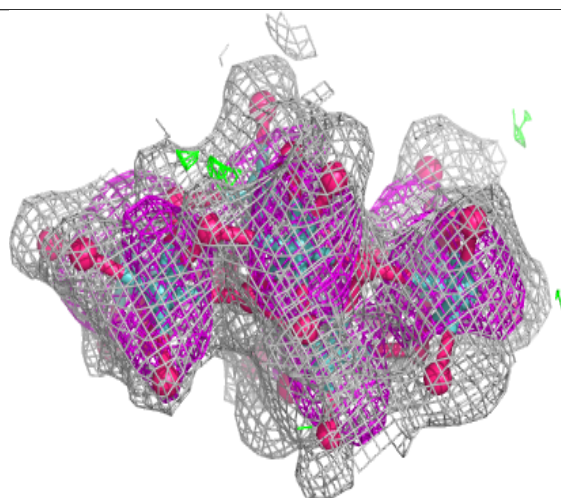
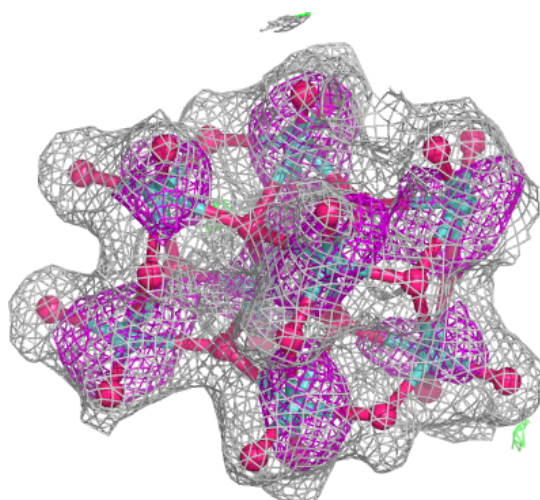
**Electron density around 8M0 C 304:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



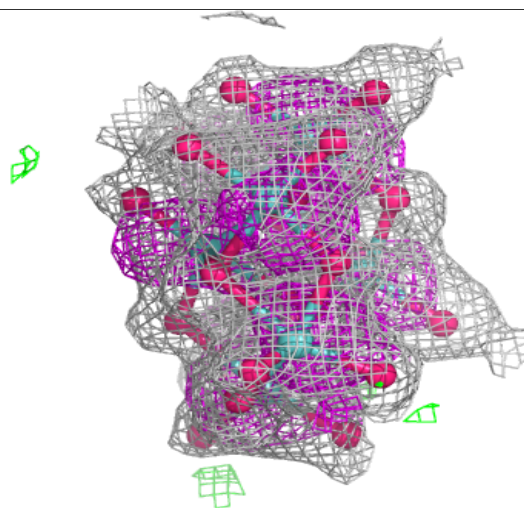
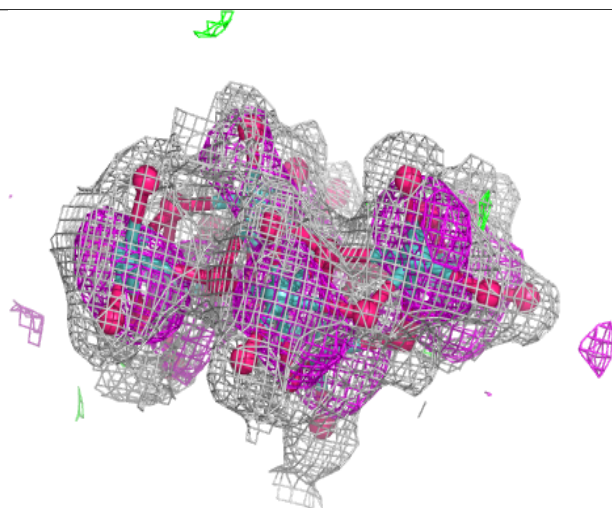
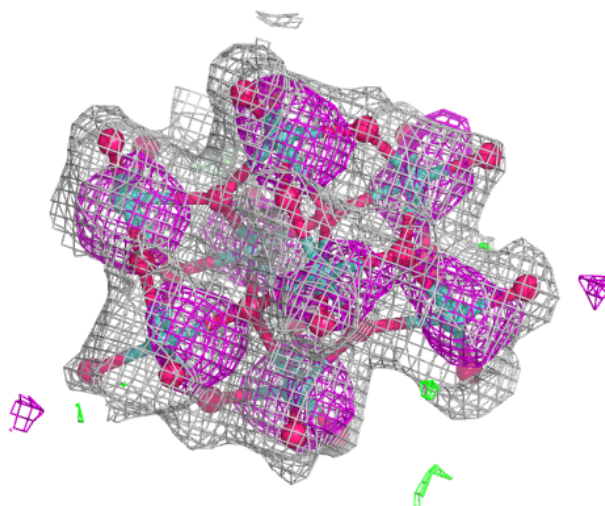
**Electron density around 8M0 G 303:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



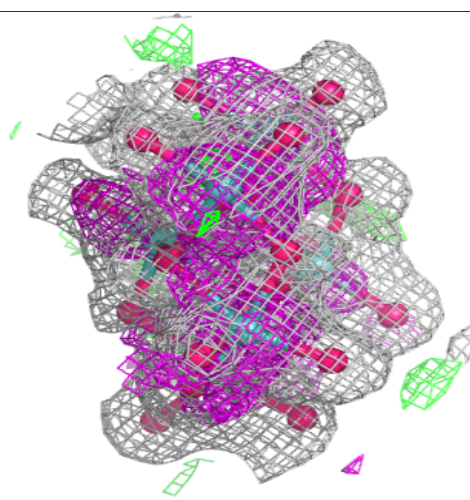
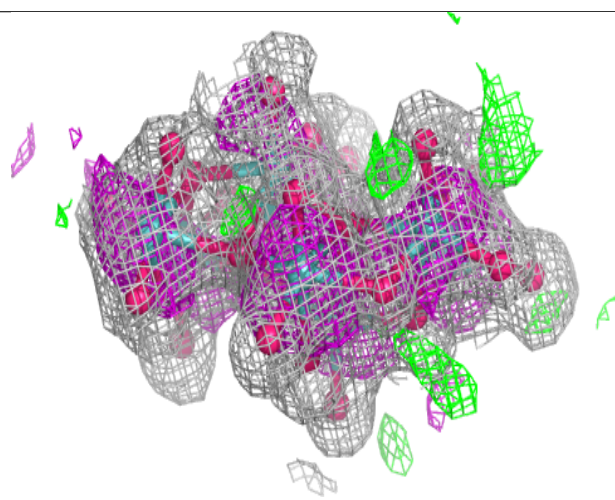
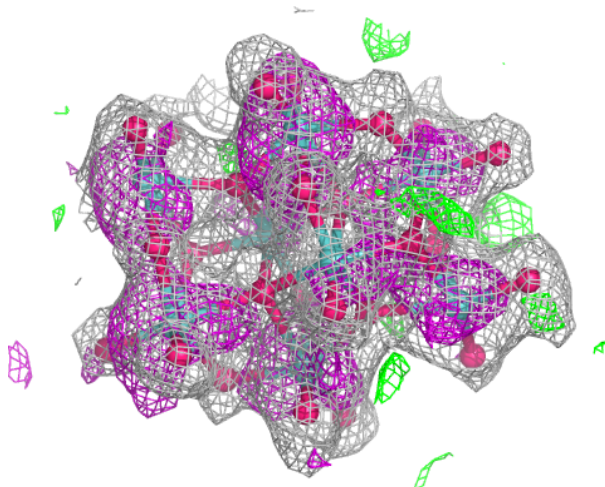
**Electron density around 8M0 I 303:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



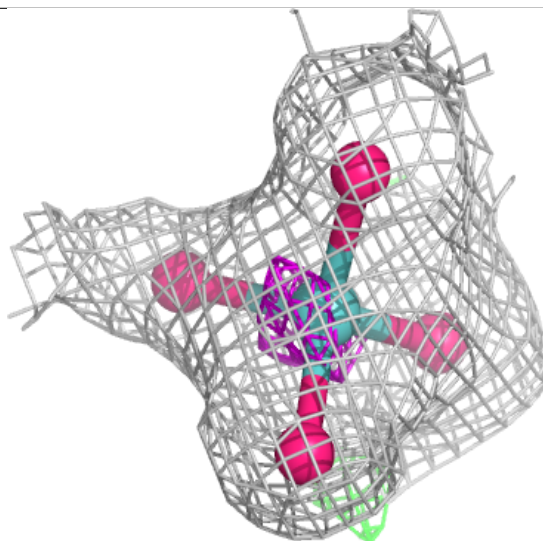
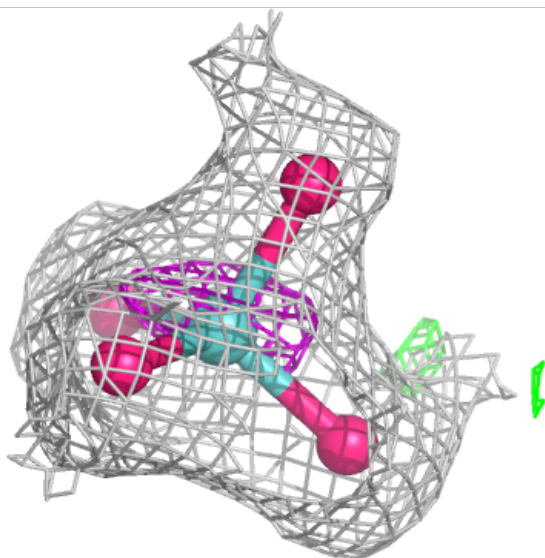
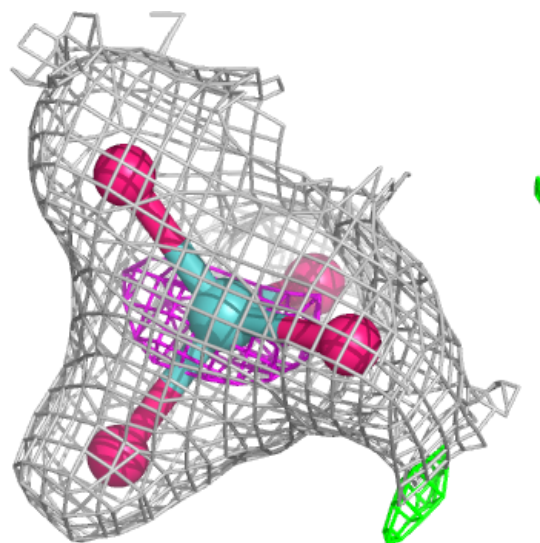
**Electron density around 8M0 A 303:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



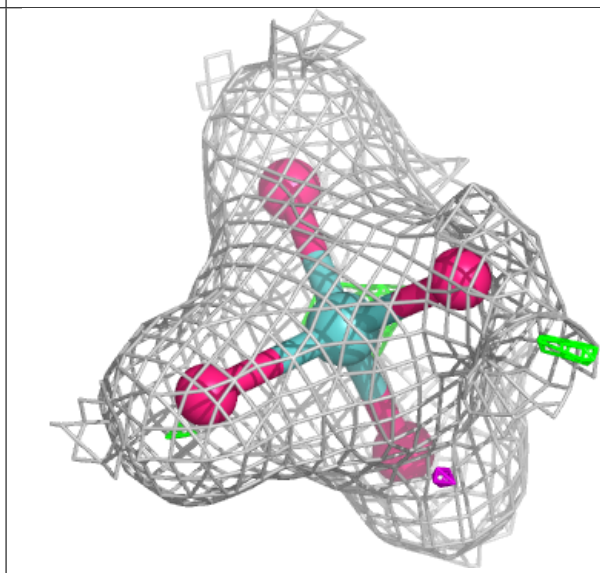
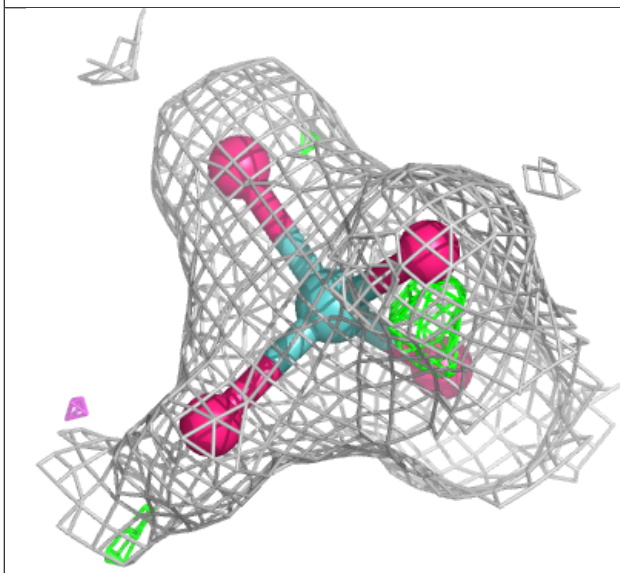
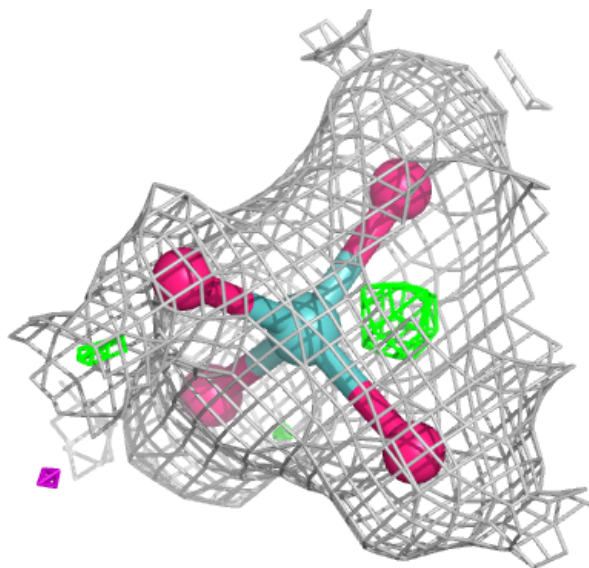
**Electron density around MOO D 303 (A):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



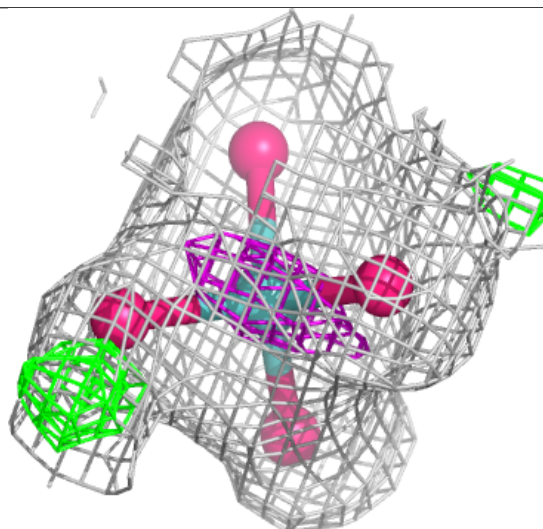
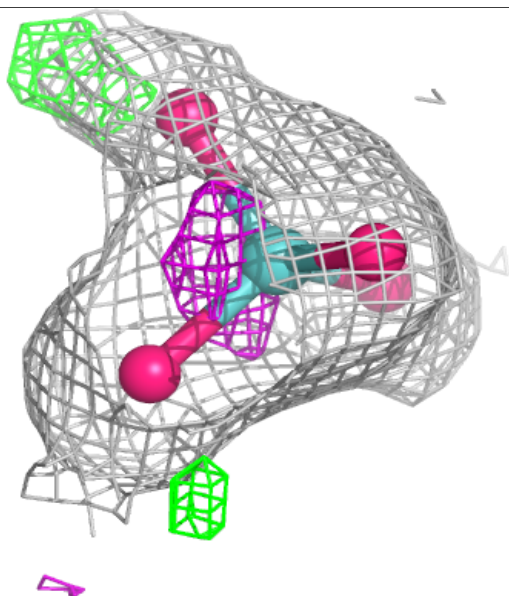
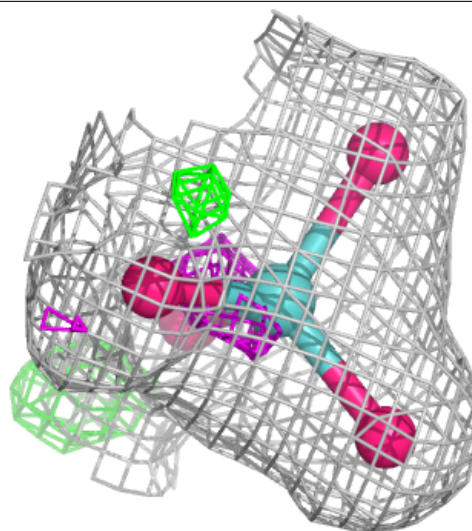
**Electron density around MOO F 304 (A):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



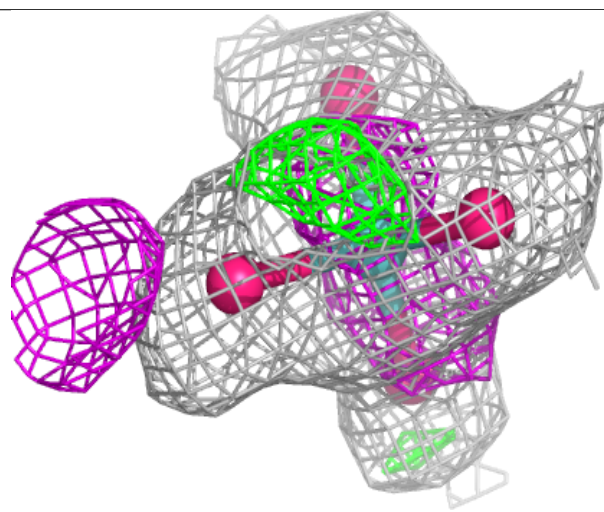
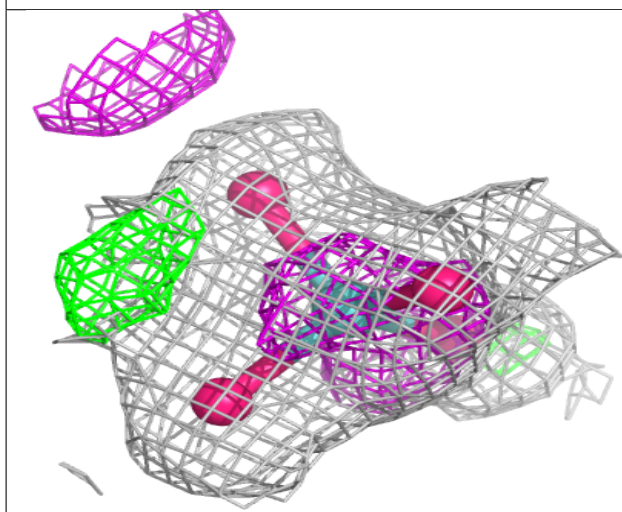
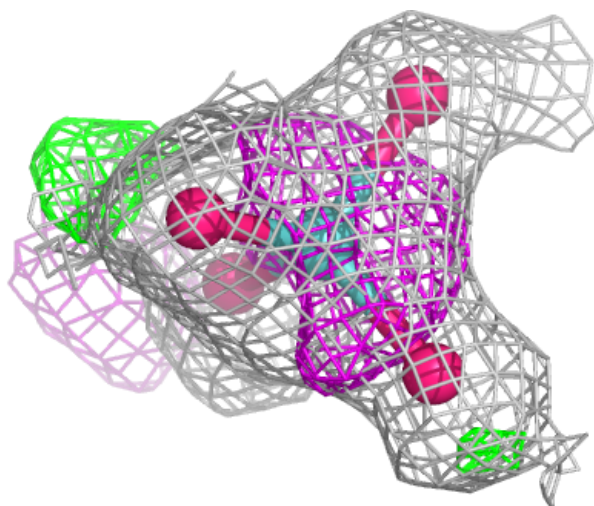
**Electron density around MOO H 304 (A):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



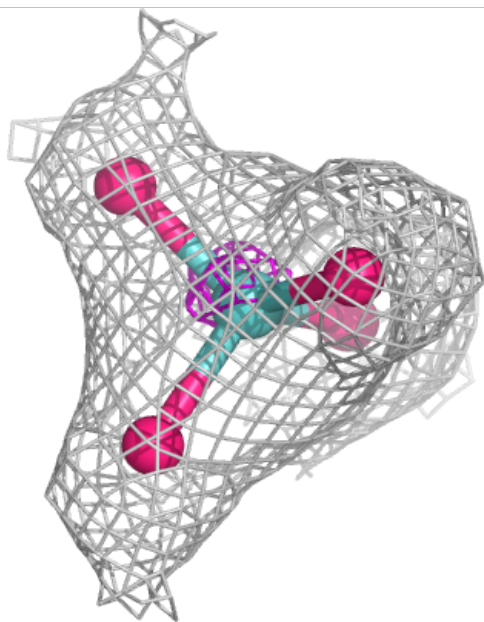
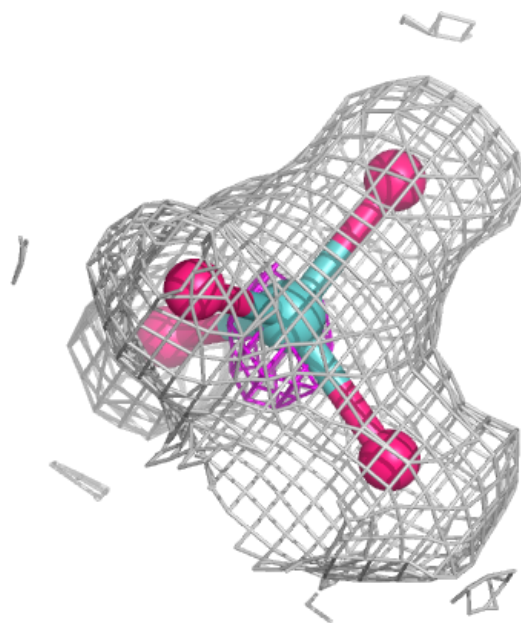
**Electron density around MOO J 304 (A):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



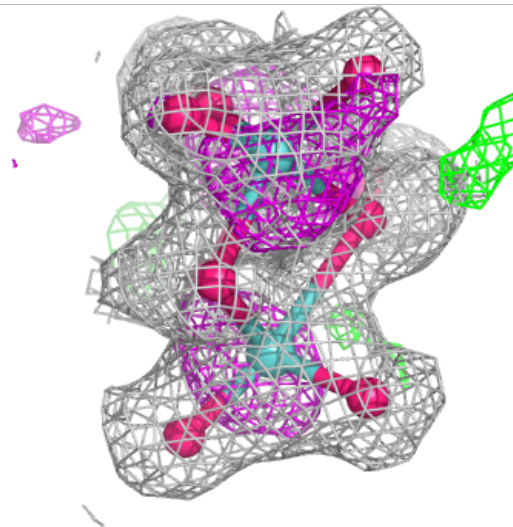
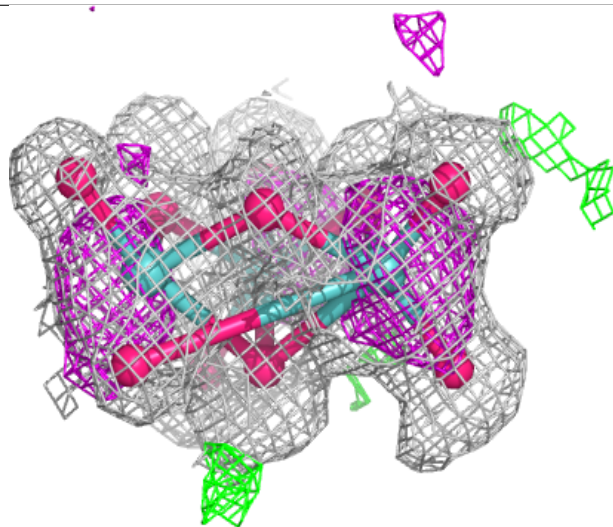
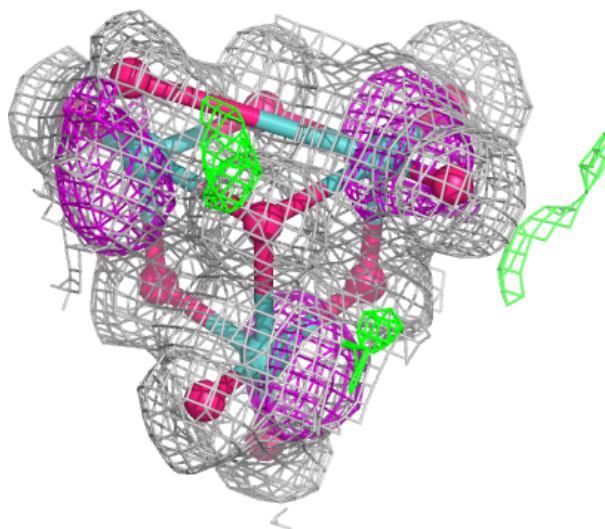
**Electron density around MOO L 304 (A):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



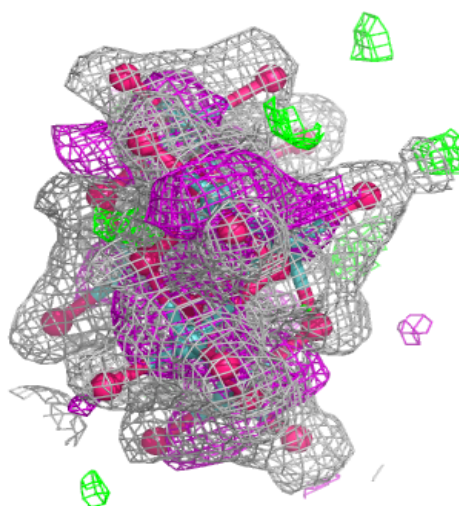
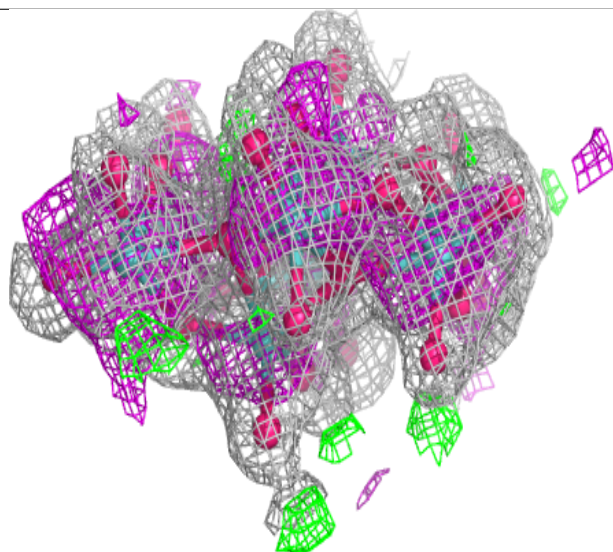
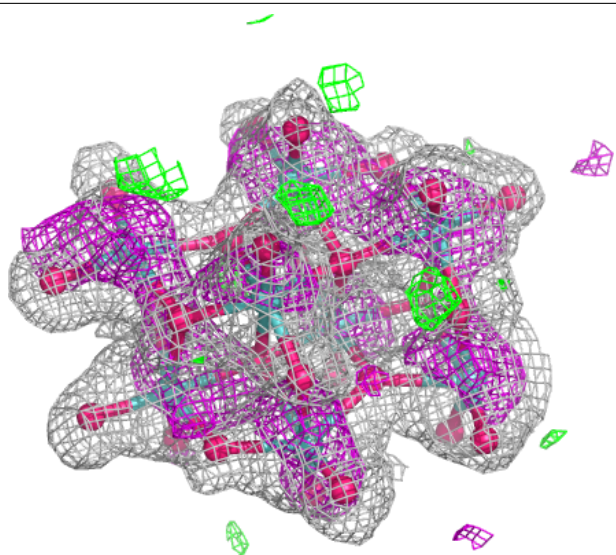
**Electron density around M10 G 304:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



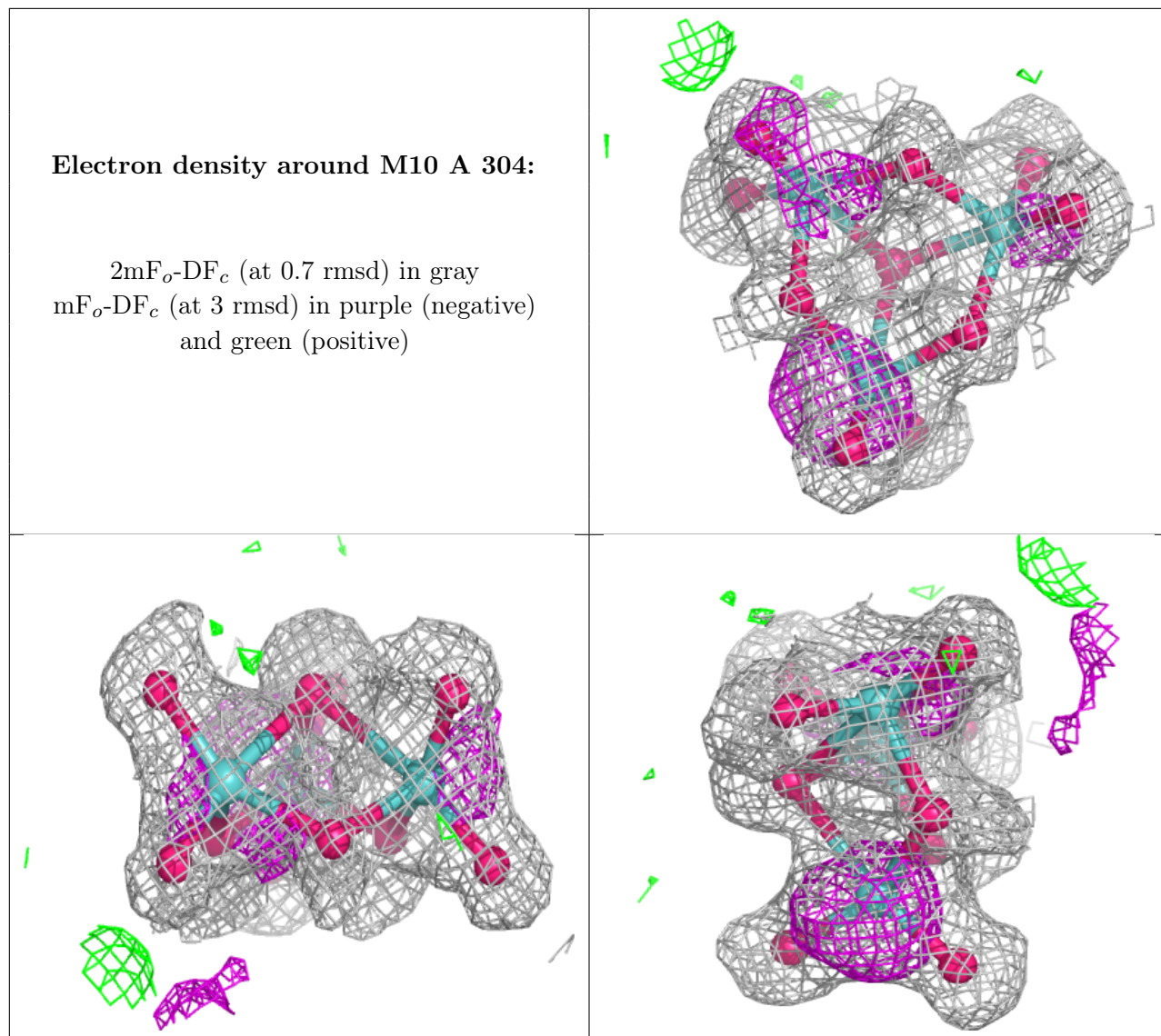
**Electron density around 8M0 E 303:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around M10 A 304:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**6.5 Other polymers** [\(i\)](#)

There are no such residues in this entry.