



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:02 AM UTC

PDB ID : 5EC5 / pdb\_00005ec5  
Title : Crystal structure of lysenin pore  
Authors : Podobnik, M.; Savory, P.; Rojko, N.; Kisovec, M.; Bruce, M.; Jayasinghe, L.;  
Anderluh, G.  
Deposited on : 2015-10-20  
Resolution : 3.10 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                                                             |

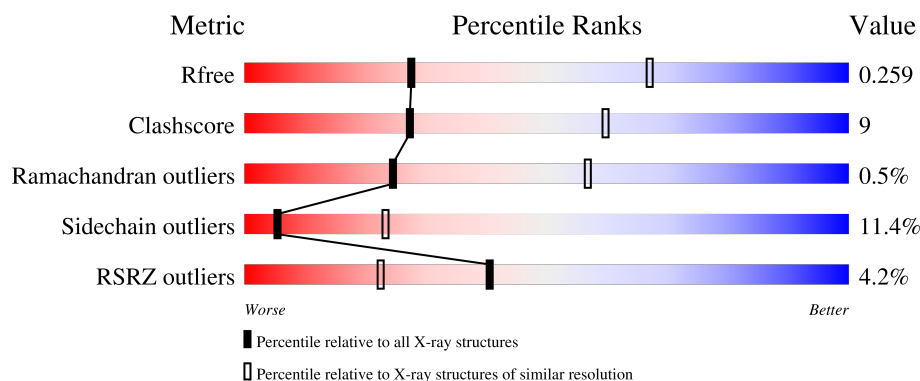
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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                      | 1456 (3.10-3.10)                                      |
| Clashscore            | 190562                      | 1539 (3.10-3.10)                                      |
| Ramachandran outliers | 187476                      | 1467 (3.10-3.10)                                      |
| Sidechain outliers    | 187428                      | 1467 (3.10-3.10)                                      |
| RSRZ outliers         | 180081                      | 1456 (3.10-3.10)                                      |

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   | A     | 298    | <div> <div>4%</div> <div>74%</div> <div>20%</div> <div>• •</div> </div>  |
| 1   | B     | 298    | <div> <div>2%</div> <div>77%</div> <div>17%</div> <div>• 5%</div> </div> |
| 1   | C     | 298    | <div> <div>6%</div> <div>73%</div> <div>21%</div> <div>• •</div> </div>  |
| 1   | D     | 298    | <div> <div>2%</div> <div>70%</div> <div>22%</div> <div>• •</div> </div>  |
| 1   | E     | 298    | <div> <div>5%</div> <div>71%</div> <div>23%</div> <div>• 5%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 298    |                  |
| 1   | G     | 298    |                  |
| 1   | H     | 298    |                  |
| 1   | I     | 298    |                  |
| 1   | J     | 298    |                  |
| 1   | K     | 298    |                  |
| 1   | L     | 298    |                  |
| 1   | M     | 298    |                  |
| 1   | N     | 298    |                  |
| 1   | O     | 298    |                  |
| 1   | P     | 298    |                  |
| 1   | R     | 298    |                  |
| 1   | S     | 298    |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | MBO  | A     | 302 | -         | -        | X       | -                |
| 2   | MBO  | B     | 301 | -         | -        | X       | -                |
| 2   | MBO  | C     | 301 | -         | -        | X       | -                |
| 2   | MBO  | D     | 301 | -         | -        | X       | -                |
| 2   | MBO  | E     | 301 | -         | -        | X       | -                |
| 2   | MBO  | F     | 302 | -         | -        | X       | -                |
| 2   | MBO  | G     | 301 | -         | -        | X       | -                |
| 2   | MBO  | H     | 301 | -         | -        | X       | -                |
| 2   | MBO  | H     | 302 | -         | -        | X       | -                |
| 2   | MBO  | I     | 302 | -         | -        | X       | -                |
| 2   | MBO  | K     | 301 | -         | -        | X       | -                |
| 2   | MBO  | K     | 302 | -         | -        | X       | -                |
| 2   | MBO  | L     | 301 | -         | -        | X       | -                |
| 2   | MBO  | L     | 302 | -         | -        | X       | -                |
| 2   | MBO  | M     | 301 | -         | -        | X       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | MBO  | O     | 301 | -         | -        | X       | -                |
| 2   | MBO  | P     | 302 | -         | -        | X       | -                |
| 2   | MBO  | R     | 301 | -         | -        | X       | -                |
| 2   | MBO  | S     | 301 | -         | -        | X       | -                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 41248 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 Lysenin.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 290      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2301  | 1459 | 390 | 444 | 8 |         |         |       |
| 1   | B     | 284      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2260  | 1432 | 384 | 436 | 8 |         |         |       |
| 1   | C     | 286      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2268  | 1436 | 386 | 438 | 8 |         |         |       |
| 1   | D     | 285      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2265  | 1435 | 385 | 437 | 8 |         |         |       |
| 1   | E     | 283      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2252  | 1428 | 383 | 433 | 8 |         |         |       |
| 1   | F     | 283      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2252  | 1428 | 383 | 433 | 8 |         |         |       |
| 1   | G     | 290      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2301  | 1459 | 390 | 444 | 8 |         |         |       |
| 1   | H     | 283      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2252  | 1428 | 383 | 433 | 8 |         |         |       |
| 1   | I     | 282      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2248  | 1426 | 382 | 432 | 8 |         |         |       |
| 1   | J     | 290      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2301  | 1459 | 390 | 444 | 8 |         |         |       |
| 1   | K     | 290      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2301  | 1459 | 390 | 444 | 8 |         |         |       |
| 1   | L     | 284      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2260  | 1434 | 384 | 434 | 8 |         |         |       |
| 1   | M     | 289      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2297  | 1457 | 389 | 443 | 8 |         |         |       |
| 1   | N     | 289      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2297  | 1457 | 389 | 443 | 8 |         |         |       |
| 1   | O     | 289      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2297  | 1457 | 389 | 443 | 8 |         |         |       |
| 1   | P     | 289      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2297  | 1457 | 389 | 443 | 8 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | R     | 283      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2252  | 1428 | 383 | 433 | 8 |         |         |       |
| 1   | S     | 283      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2252  | 1428 | 383 | 433 | 8 |         |         |       |

There are 108 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 0       | GLY      | -      | expression tag      | UNP O18423 |
| A     | 84      | GLN      | GLU    | engineered mutation | UNP O18423 |
| A     | 85      | LYS      | GLU    | engineered mutation | UNP O18423 |
| A     | 92      | GLN      | GLU    | engineered mutation | UNP O18423 |
| A     | 97      | SER      | GLU    | engineered mutation | UNP O18423 |
| A     | 126     | GLY      | ASP    | engineered mutation | UNP O18423 |
| B     | 0       | GLY      | -      | expression tag      | UNP O18423 |
| B     | 84      | GLN      | GLU    | engineered mutation | UNP O18423 |
| B     | 85      | LYS      | GLU    | engineered mutation | UNP O18423 |
| B     | 92      | GLN      | GLU    | engineered mutation | UNP O18423 |
| B     | 97      | SER      | GLU    | engineered mutation | UNP O18423 |
| B     | 126     | GLY      | ASP    | engineered mutation | UNP O18423 |
| C     | 0       | GLY      | -      | expression tag      | UNP O18423 |
| C     | 84      | GLN      | GLU    | engineered mutation | UNP O18423 |
| C     | 85      | LYS      | GLU    | engineered mutation | UNP O18423 |
| C     | 92      | GLN      | GLU    | engineered mutation | UNP O18423 |
| C     | 97      | SER      | GLU    | engineered mutation | UNP O18423 |
| C     | 126     | GLY      | ASP    | engineered mutation | UNP O18423 |
| D     | 0       | GLY      | -      | expression tag      | UNP O18423 |
| D     | 84      | GLN      | GLU    | engineered mutation | UNP O18423 |
| D     | 85      | LYS      | GLU    | engineered mutation | UNP O18423 |
| D     | 92      | GLN      | GLU    | engineered mutation | UNP O18423 |
| D     | 97      | SER      | GLU    | engineered mutation | UNP O18423 |
| D     | 126     | GLY      | ASP    | engineered mutation | UNP O18423 |
| E     | 0       | GLY      | -      | expression tag      | UNP O18423 |
| E     | 84      | GLN      | GLU    | engineered mutation | UNP O18423 |
| E     | 85      | LYS      | GLU    | engineered mutation | UNP O18423 |
| E     | 92      | GLN      | GLU    | engineered mutation | UNP O18423 |
| E     | 97      | SER      | GLU    | engineered mutation | UNP O18423 |
| E     | 126     | GLY      | ASP    | engineered mutation | UNP O18423 |
| F     | 0       | GLY      | -      | expression tag      | UNP O18423 |
| F     | 84      | GLN      | GLU    | engineered mutation | UNP O18423 |
| F     | 85      | LYS      | GLU    | engineered mutation | UNP O18423 |
| F     | 92      | GLN      | GLU    | engineered mutation | UNP O18423 |

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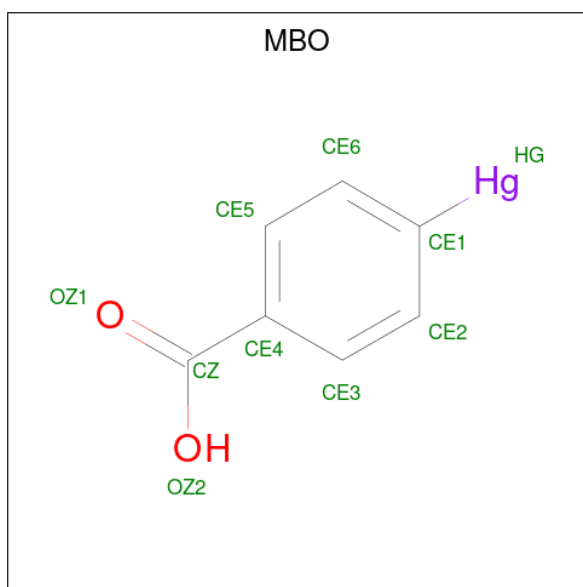
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| F     | 97      | SER      | GLU    | engineered mutation | UNP O18423 |
| F     | 126     | GLY      | ASP    | engineered mutation | UNP O18423 |
| G     | 0       | GLY      | -      | expression tag      | UNP O18423 |
| G     | 84      | GLN      | GLU    | engineered mutation | UNP O18423 |
| G     | 85      | LYS      | GLU    | engineered mutation | UNP O18423 |
| G     | 92      | GLN      | GLU    | engineered mutation | UNP O18423 |
| G     | 97      | SER      | GLU    | engineered mutation | UNP O18423 |
| G     | 126     | GLY      | ASP    | engineered mutation | UNP O18423 |
| H     | 0       | GLY      | -      | expression tag      | UNP O18423 |
| H     | 84      | GLN      | GLU    | engineered mutation | UNP O18423 |
| H     | 85      | LYS      | GLU    | engineered mutation | UNP O18423 |
| H     | 92      | GLN      | GLU    | engineered mutation | UNP O18423 |
| H     | 97      | SER      | GLU    | engineered mutation | UNP O18423 |
| H     | 126     | GLY      | ASP    | engineered mutation | UNP O18423 |
| I     | 0       | GLY      | -      | expression tag      | UNP O18423 |
| I     | 84      | GLN      | GLU    | engineered mutation | UNP O18423 |
| I     | 85      | LYS      | GLU    | engineered mutation | UNP O18423 |
| I     | 92      | GLN      | GLU    | engineered mutation | UNP O18423 |
| I     | 97      | SER      | GLU    | engineered mutation | UNP O18423 |
| I     | 126     | GLY      | ASP    | engineered mutation | UNP O18423 |
| J     | 0       | GLY      | -      | expression tag      | UNP O18423 |
| J     | 84      | GLN      | GLU    | engineered mutation | UNP O18423 |
| J     | 85      | LYS      | GLU    | engineered mutation | UNP O18423 |
| J     | 92      | GLN      | GLU    | engineered mutation | UNP O18423 |
| J     | 97      | SER      | GLU    | engineered mutation | UNP O18423 |
| J     | 126     | GLY      | ASP    | engineered mutation | UNP O18423 |
| K     | 0       | GLY      | -      | expression tag      | UNP O18423 |
| K     | 84      | GLN      | GLU    | engineered mutation | UNP O18423 |
| K     | 85      | LYS      | GLU    | engineered mutation | UNP O18423 |
| K     | 92      | GLN      | GLU    | engineered mutation | UNP O18423 |
| K     | 97      | SER      | GLU    | engineered mutation | UNP O18423 |
| K     | 126     | GLY      | ASP    | engineered mutation | UNP O18423 |
| L     | 0       | GLY      | -      | expression tag      | UNP O18423 |
| L     | 84      | GLN      | GLU    | engineered mutation | UNP O18423 |
| L     | 85      | LYS      | GLU    | engineered mutation | UNP O18423 |
| L     | 92      | GLN      | GLU    | engineered mutation | UNP O18423 |
| L     | 97      | SER      | GLU    | engineered mutation | UNP O18423 |
| L     | 126     | GLY      | ASP    | engineered mutation | UNP O18423 |
| M     | 0       | GLY      | -      | expression tag      | UNP O18423 |
| M     | 84      | GLN      | GLU    | engineered mutation | UNP O18423 |
| M     | 85      | LYS      | GLU    | engineered mutation | UNP O18423 |
| M     | 92      | GLN      | GLU    | engineered mutation | UNP O18423 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| M     | 97      | SER      | GLU    | engineered mutation | UNP O18423 |
| M     | 126     | GLY      | ASP    | engineered mutation | UNP O18423 |
| N     | 0       | GLY      | -      | expression tag      | UNP O18423 |
| N     | 84      | GLN      | GLU    | engineered mutation | UNP O18423 |
| N     | 85      | LYS      | GLU    | engineered mutation | UNP O18423 |
| N     | 92      | GLN      | GLU    | engineered mutation | UNP O18423 |
| N     | 97      | SER      | GLU    | engineered mutation | UNP O18423 |
| N     | 126     | GLY      | ASP    | engineered mutation | UNP O18423 |
| O     | 0       | GLY      | -      | expression tag      | UNP O18423 |
| O     | 84      | GLN      | GLU    | engineered mutation | UNP O18423 |
| O     | 85      | LYS      | GLU    | engineered mutation | UNP O18423 |
| O     | 92      | GLN      | GLU    | engineered mutation | UNP O18423 |
| O     | 97      | SER      | GLU    | engineered mutation | UNP O18423 |
| O     | 126     | GLY      | ASP    | engineered mutation | UNP O18423 |
| P     | 0       | GLY      | -      | expression tag      | UNP O18423 |
| P     | 84      | GLN      | GLU    | engineered mutation | UNP O18423 |
| P     | 85      | LYS      | GLU    | engineered mutation | UNP O18423 |
| P     | 92      | GLN      | GLU    | engineered mutation | UNP O18423 |
| P     | 97      | SER      | GLU    | engineered mutation | UNP O18423 |
| P     | 126     | GLY      | ASP    | engineered mutation | UNP O18423 |
| R     | 0       | GLY      | -      | expression tag      | UNP O18423 |
| R     | 84      | GLN      | GLU    | engineered mutation | UNP O18423 |
| R     | 85      | LYS      | GLU    | engineered mutation | UNP O18423 |
| R     | 92      | GLN      | GLU    | engineered mutation | UNP O18423 |
| R     | 97      | SER      | GLU    | engineered mutation | UNP O18423 |
| R     | 126     | GLY      | ASP    | engineered mutation | UNP O18423 |
| S     | 0       | GLY      | -      | expression tag      | UNP O18423 |
| S     | 84      | GLN      | GLU    | engineered mutation | UNP O18423 |
| S     | 85      | LYS      | GLU    | engineered mutation | UNP O18423 |
| S     | 92      | GLN      | GLU    | engineered mutation | UNP O18423 |
| S     | 97      | SER      | GLU    | engineered mutation | UNP O18423 |
| S     | 126     | GLY      | ASP    | engineered mutation | UNP O18423 |

- Molecule 2 is MERCURIBENZOIC ACID (CCD ID: MBO) (formula: C<sub>7</sub>H<sub>5</sub>HgO<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 2   | A     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | A     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | B     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | B     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | C     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | D     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | E     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | F     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | G     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | H     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | H     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | I     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | K     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | K     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |

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| Mol | Chain | Residues | Atoms |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 2   | L     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | L     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | M     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | M     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | O     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | P     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | R     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |
| 2   | S     | 1        | Total | C | Hg | O | 0       | 0       |
|     |       |          | 10    | 7 | 1  | 2 |         |         |

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | C     | 1        | Total | Hg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | D     | 1        | Total | Hg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | E     | 1        | Total | Hg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | F     | 1        | Total | Hg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | G     | 1        | Total | Hg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | I     | 1        | Total | Hg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | J     | 2        | Total | Hg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 3   | N     | 2        | Total | Hg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 3   | O     | 1        | Total | Hg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | P     | 1        | Total | Hg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | R     | 1        | Total | Hg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | S     | 1        | Total | Hg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

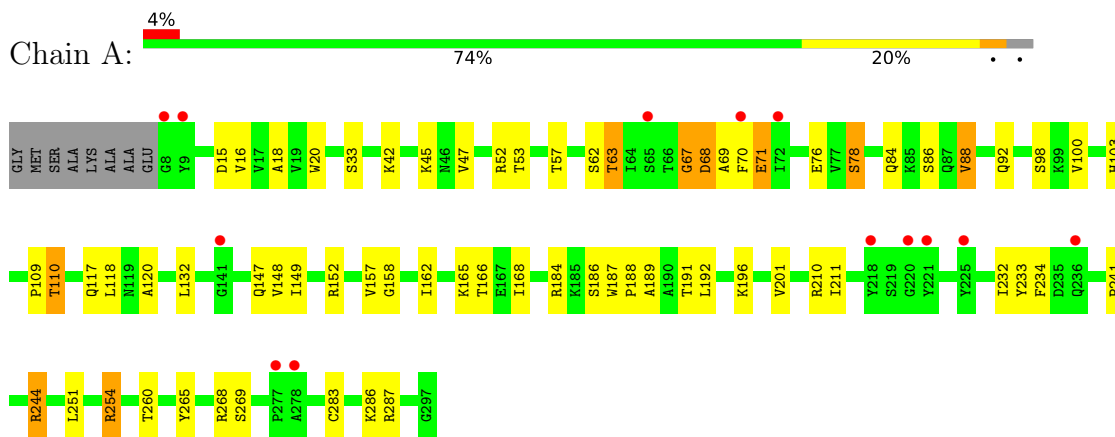
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 4   | A     | 7        | Total | O | 0       | 0       |
|     |       |          | 7     | 7 |         |         |
| 4   | B     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 4   | C     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 4   | D     | 7        | Total | O | 0       | 0       |
|     |       |          | 7     | 7 |         |         |
| 4   | E     | 5        | Total | O | 0       | 0       |
|     |       |          | 5     | 5 |         |         |
| 4   | F     | 5        | Total | O | 0       | 0       |
|     |       |          | 5     | 5 |         |         |
| 4   | G     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 4   | H     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 4   | I     | 4        | Total | O | 0       | 0       |
|     |       |          | 4     | 4 |         |         |
| 4   | J     | 4        | Total | O | 0       | 0       |
|     |       |          | 4     | 4 |         |         |
| 4   | K     | 8        | Total | O | 0       | 0       |
|     |       |          | 8     | 8 |         |         |
| 4   | L     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 4   | M     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 4   | N     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 4   | O     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 4   | P     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 4   | R     | 3        | Total | O | 0       | 0       |
|     |       |          | 3     | 3 |         |         |
| 4   | S     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

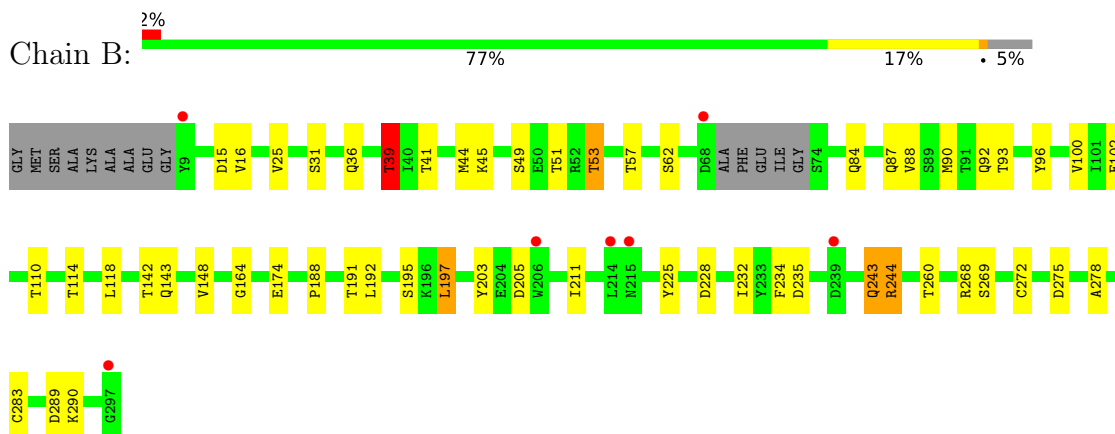
### 3 Residue-property plots [i](#)

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.

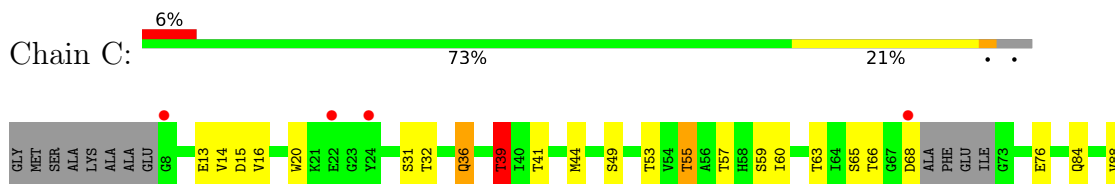
#### • Molecule 1: Lysenin

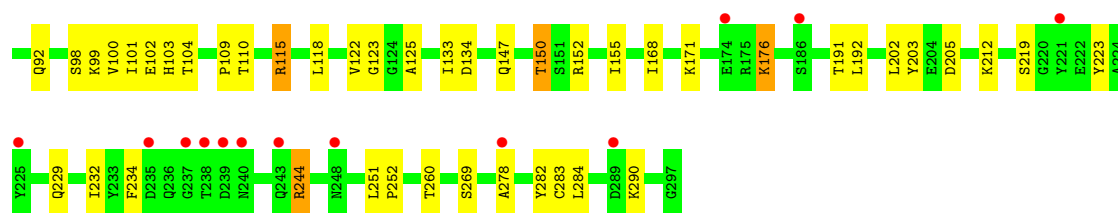


#### • Molecule 1: Lysenin

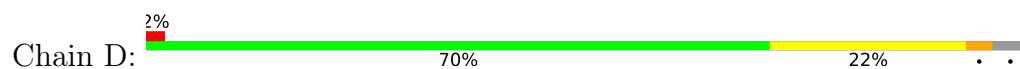


#### • Molecule 1: Lysenin

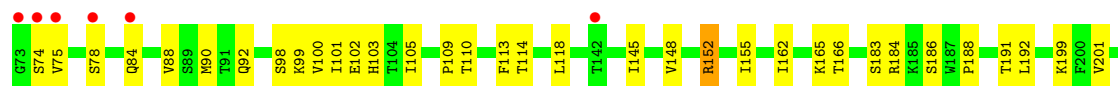




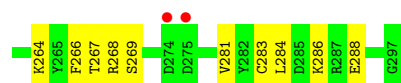
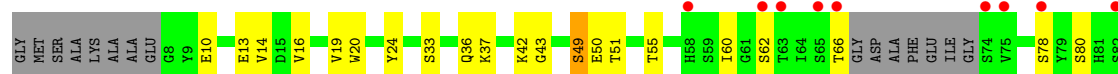
• Molecule 1: Lysenin



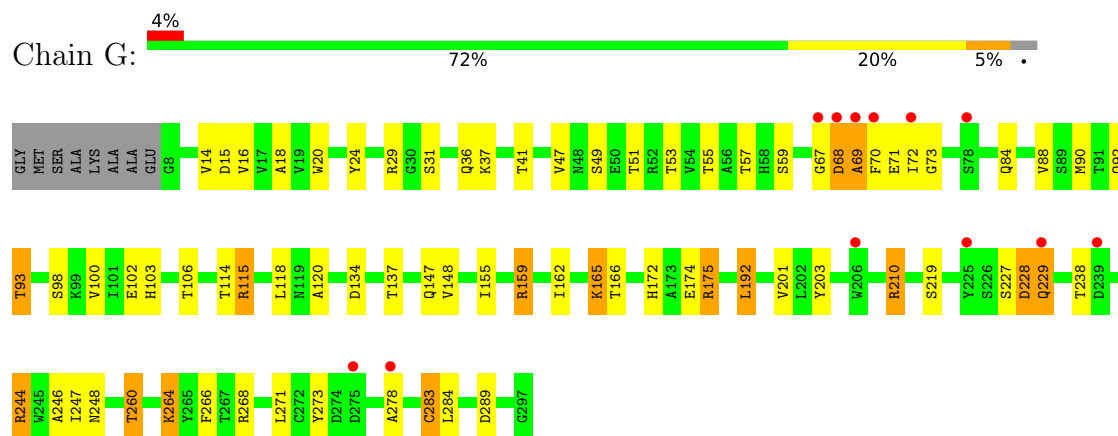
• Molecule 1: Lysenin



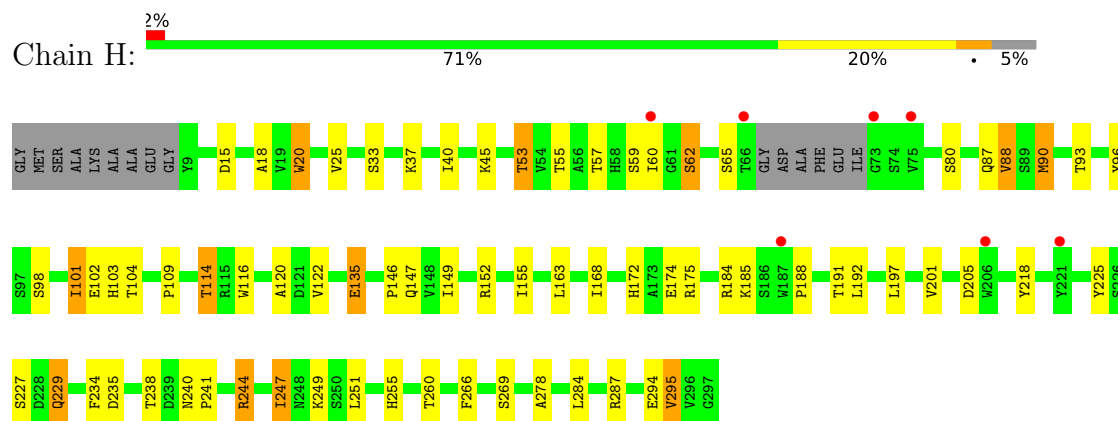
• Molecule 1: Lysenin



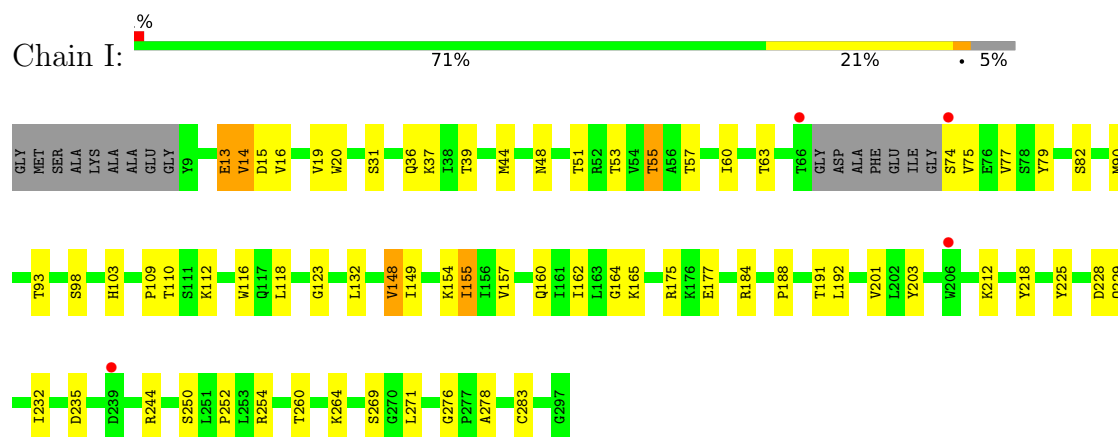
- Molecule 1: Lysenin



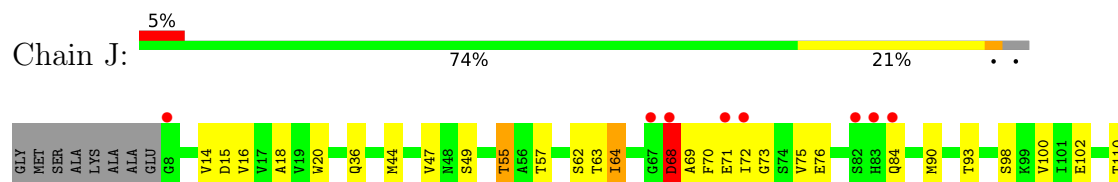
- Molecule 1: Lysenin

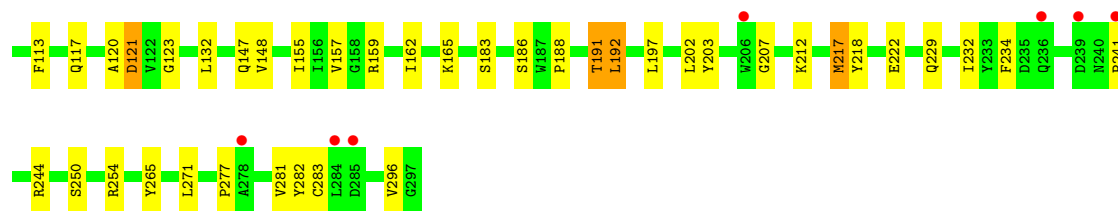


- Molecule 1: Lysenin

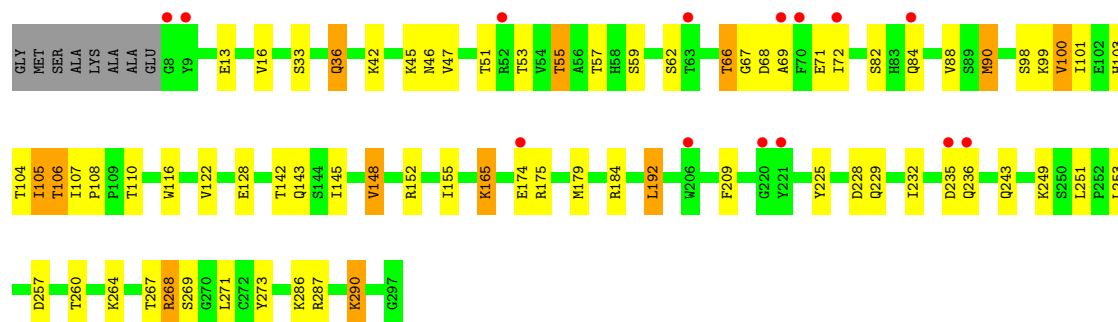
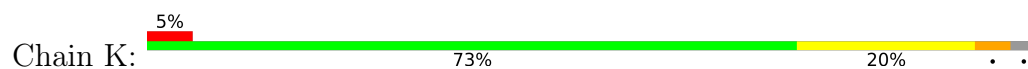


- Molecule 1: Lysenin

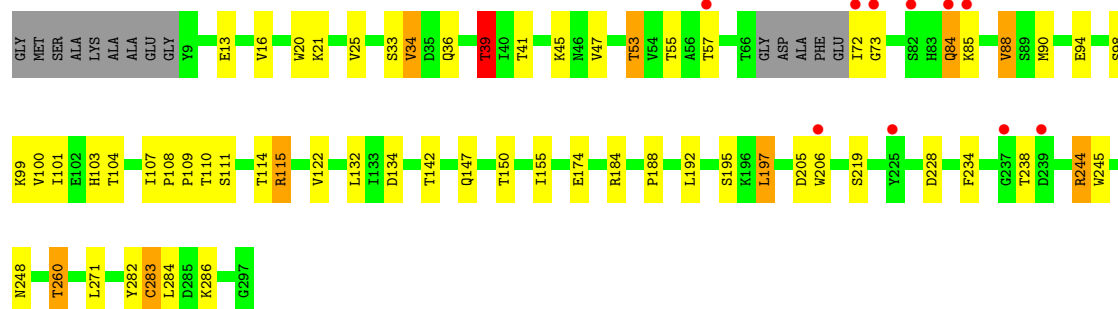
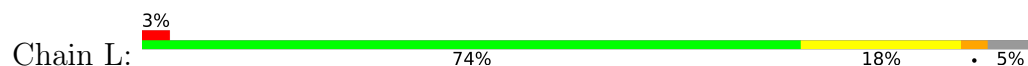




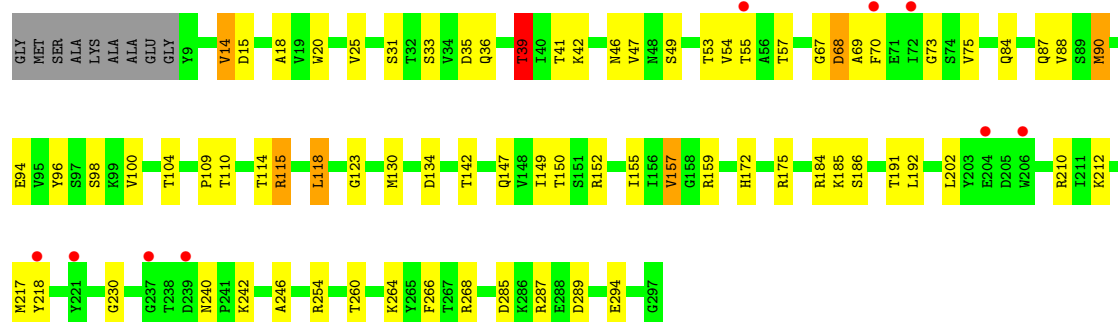
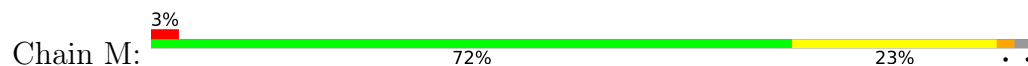
• Molecule 1: Lysenin



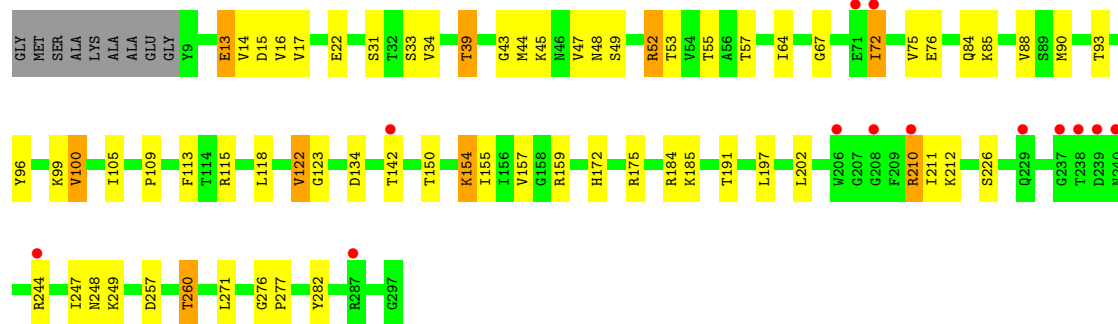
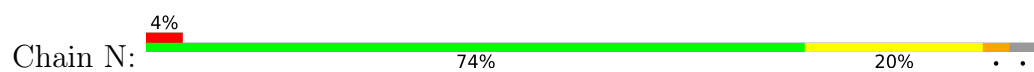
• Molecule 1: Lysenin



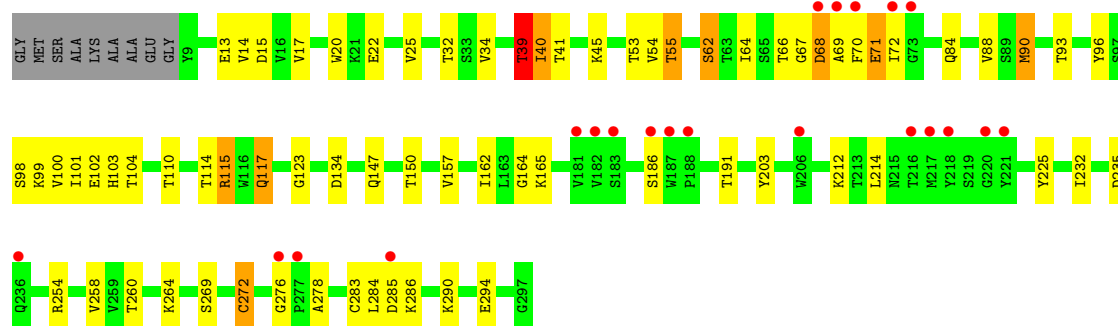
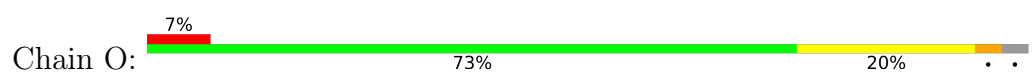
• Molecule 1: Lysenin



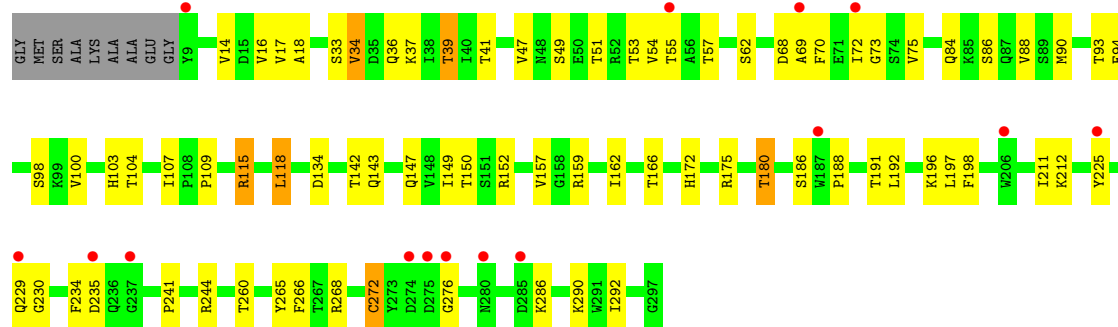
• Molecule 1: Lysenin



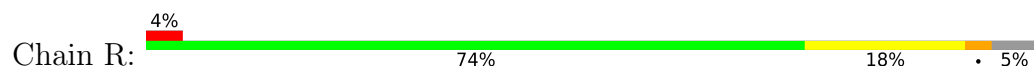
• Molecule 1: Lysenin

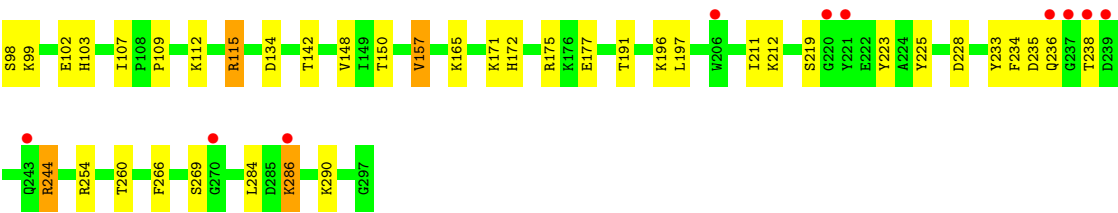


• Molecule 1: Lysenin

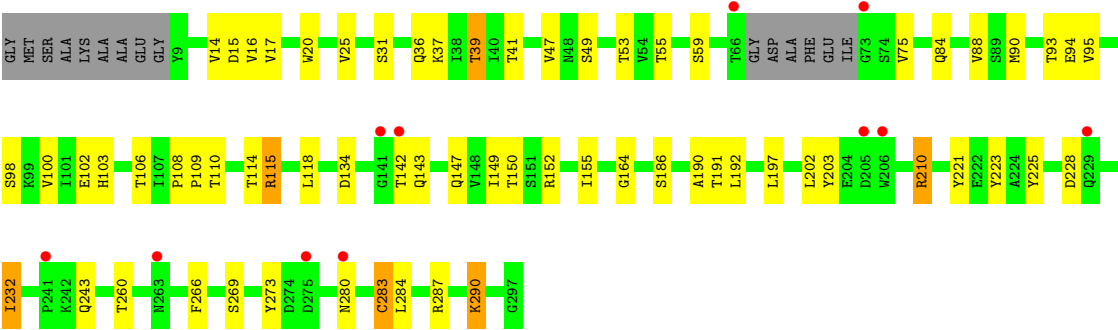


• Molecule 1: Lysenin





● Molecule 1: Lysenin



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 43 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 192.99Å 192.99Å 493.20Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.10 – 3.10<br>49.10 – 3.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (49.10-3.10)<br>99.9 (49.10-3.10)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.20                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.61 (at 3.12Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0103                                             | Depositor        |
| R, $R_{free}$                                                           | 0.214 , 0.258<br>0.218 , 0.259                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 8448 reflections (5.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 57.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.541                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 45.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 41248                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 57.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.61% 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: HG, MBO

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.66         | 0/2352      | 0.96        | 2/3186 (0.1%)   |
| 1   | B     | 0.62         | 0/2309      | 0.89        | 1/3127 (0.0%)   |
| 1   | C     | 0.65         | 0/2317      | 0.89        | 2/3137 (0.1%)   |
| 1   | D     | 0.64         | 0/2314      | 0.92        | 2/3133 (0.1%)   |
| 1   | E     | 0.66         | 0/2301      | 0.92        | 2/3116 (0.1%)   |
| 1   | F     | 0.73         | 0/2301      | 0.99        | 2/3116 (0.1%)   |
| 1   | G     | 0.71         | 0/2352      | 1.00        | 6/3186 (0.2%)   |
| 1   | H     | 0.66         | 0/2301      | 0.96        | 2/3116 (0.1%)   |
| 1   | I     | 0.67         | 0/2297      | 0.95        | 2/3111 (0.1%)   |
| 1   | J     | 0.65         | 0/2352      | 0.92        | 1/3186 (0.0%)   |
| 1   | K     | 0.67         | 0/2352      | 0.99        | 4/3186 (0.1%)   |
| 1   | L     | 0.62         | 0/2309      | 0.91        | 2/3127 (0.1%)   |
| 1   | M     | 0.66         | 0/2348      | 0.90        | 1/3181 (0.0%)   |
| 1   | N     | 0.65         | 0/2348      | 0.92        | 3/3181 (0.1%)   |
| 1   | O     | 0.66         | 0/2348      | 0.94        | 5/3181 (0.2%)   |
| 1   | P     | 0.67         | 0/2348      | 0.95        | 2/3181 (0.1%)   |
| 1   | R     | 0.65         | 0/2301      | 0.92        | 3/3116 (0.1%)   |
| 1   | S     | 0.63         | 0/2301      | 0.91        | 1/3116 (0.0%)   |
| All | All   | 0.66         | 0/41851     | 0.94        | 43/56683 (0.1%) |

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   | A     | 0                   | 1                   |
| 1   | S     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

There are no bond length outliers.

All (43) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | K     | 106 | THR  | CB-CA-C | 7.80  | 123.50      | 110.79   |
| 1   | G     | 73  | GLY  | N-CA-C  | -6.62 | 102.02      | 111.42   |
| 1   | H     | 101 | ILE  | CB-CA-C | 6.32  | 118.71      | 110.12   |
| 1   | O     | 68  | ASP  | N-CA-C  | 6.17  | 123.95      | 110.80   |
| 1   | O     | 71  | GLU  | N-CA-C  | -6.12 | 97.77       | 110.80   |
| 1   | K     | 148 | VAL  | N-CA-C  | 5.95  | 116.42      | 108.27   |
| 1   | D     | 39  | THR  | CB-CA-C | 5.92  | 119.26      | 110.14   |
| 1   | R     | 107 | ILE  | CA-C-N  | 5.91  | 126.47      | 120.38   |
| 1   | R     | 107 | ILE  | C-N-CA  | 5.91  | 126.47      | 120.38   |
| 1   | M     | 39  | THR  | CB-CA-C | 5.88  | 119.21      | 110.62   |
| 1   | L     | 150 | THR  | CB-CA-C | 5.86  | 118.79      | 110.24   |
| 1   | F     | 60  | ILE  | CB-CA-C | 5.82  | 118.03      | 110.12   |
| 1   | O     | 276 | GLY  | CA-C-N  | 5.75  | 125.88      | 119.32   |
| 1   | O     | 276 | GLY  | C-N-CA  | 5.75  | 125.88      | 119.32   |
| 1   | C     | 150 | THR  | CB-CA-C | 5.73  | 121.01      | 109.38   |
| 1   | G     | 68  | ASP  | N-CA-C  | 5.71  | 122.97      | 110.80   |
| 1   | N     | 142 | THR  | CB-CA-C | 5.48  | 118.90      | 110.14   |
| 1   | S     | 142 | THR  | N-CA-C  | 5.46  | 119.56      | 111.87   |
| 1   | N     | 276 | GLY  | CA-C-N  | 5.40  | 124.86      | 119.24   |
| 1   | N     | 276 | GLY  | C-N-CA  | 5.40  | 124.86      | 119.24   |
| 1   | C     | 39  | THR  | CB-CA-C | 5.37  | 118.46      | 110.62   |
| 1   | J     | 121 | ASP  | CB-CA-C | 5.34  | 118.96      | 109.72   |
| 1   | G     | 69  | ALA  | N-CA-C  | 5.33  | 118.24      | 109.76   |
| 1   | G     | 137 | THR  | CA-C-N  | -5.32 | 114.76      | 120.03   |
| 1   | G     | 137 | THR  | C-N-CA  | -5.32 | 114.76      | 120.03   |
| 1   | O     | 39  | THR  | CB-CA-C | 5.29  | 118.28      | 110.14   |
| 1   | I     | 276 | GLY  | CA-C-N  | 5.26  | 124.44      | 118.97   |
| 1   | I     | 276 | GLY  | C-N-CA  | 5.26  | 124.44      | 118.97   |
| 1   | B     | 39  | THR  | CB-CA-C | 5.22  | 118.24      | 110.62   |
| 1   | H     | 135 | GLU  | N-CA-C  | 5.21  | 117.17      | 108.99   |
| 1   | E     | 74  | SER  | N-CA-C  | 5.20  | 117.28      | 109.23   |
| 1   | F     | 43  | GLY  | N-CA-C  | 5.19  | 118.28      | 110.18   |
| 1   | R     | 40  | ILE  | N-CA-C  | 5.19  | 115.44      | 108.17   |
| 1   | L     | 39  | THR  | CB-CA-C | 5.17  | 118.16      | 110.62   |
| 1   | K     | 165 | LYS  | N-CA-C  | 5.14  | 119.30      | 112.72   |
| 1   | G     | 166 | THR  | CB-CA-C | -5.12 | 102.58      | 110.26   |
| 1   | K     | 267 | THR  | N-CA-C  | 5.12  | 116.86      | 111.28   |
| 1   | E     | 49  | SER  | N-CA-C  | 5.08  | 117.11      | 109.23   |
| 1   | A     | 187 | TRP  | CA-C-N  | -5.07 | 114.40      | 120.13   |
| 1   | A     | 187 | TRP  | C-N-CA  | -5.07 | 114.40      | 120.13   |
| 1   | D     | 259 | VAL  | N-CA-C  | 5.06  | 116.15      | 108.96   |
| 1   | P     | 272 | CYS  | N-CA-C  | 5.06  | 115.72      | 108.74   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | P     | 73  | GLY  | N-CA-C | 5.03 | 118.56      | 111.42   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 67  | GLY  | Peptide |
| 1   | S     | 221 | TYR  | 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   | A     | 2301  | 0        | 2264     | 33      | 0            |
| 1   | B     | 2260  | 0        | 2226     | 26      | 0            |
| 1   | C     | 2268  | 0        | 2233     | 32      | 0            |
| 1   | D     | 2265  | 0        | 2232     | 42      | 0            |
| 1   | E     | 2252  | 0        | 2222     | 35      | 0            |
| 1   | F     | 2252  | 0        | 2222     | 34      | 1            |
| 1   | G     | 2301  | 0        | 2265     | 52      | 0            |
| 1   | H     | 2252  | 0        | 2223     | 50      | 0            |
| 1   | I     | 2248  | 0        | 2219     | 30      | 0            |
| 1   | J     | 2301  | 0        | 2265     | 27      | 0            |
| 1   | K     | 2301  | 0        | 2265     | 33      | 0            |
| 1   | L     | 2260  | 0        | 2234     | 39      | 0            |
| 1   | M     | 2297  | 0        | 2262     | 47      | 0            |
| 1   | N     | 2297  | 0        | 2262     | 38      | 0            |
| 1   | O     | 2297  | 0        | 2262     | 40      | 0            |
| 1   | P     | 2297  | 0        | 2261     | 36      | 0            |
| 1   | R     | 2252  | 0        | 2222     | 35      | 1            |
| 1   | S     | 2252  | 0        | 2223     | 33      | 0            |
| 2   | A     | 20    | 0        | 8        | 9       | 0            |
| 2   | B     | 20    | 0        | 8        | 16      | 0            |
| 2   | C     | 10    | 0        | 4        | 10      | 0            |
| 2   | D     | 10    | 0        | 4        | 17      | 0            |
| 2   | E     | 10    | 0        | 4        | 6       | 0            |
| 2   | F     | 10    | 0        | 4        | 19      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | G     | 10    | 0        | 4        | 13      | 0            |
| 2   | H     | 20    | 0        | 8        | 29      | 0            |
| 2   | I     | 10    | 0        | 4        | 6       | 0            |
| 2   | K     | 20    | 0        | 8        | 30      | 0            |
| 2   | L     | 20    | 0        | 8        | 25      | 0            |
| 2   | M     | 20    | 0        | 8        | 18      | 0            |
| 2   | O     | 10    | 0        | 4        | 13      | 0            |
| 2   | P     | 10    | 0        | 4        | 20      | 0            |
| 2   | R     | 10    | 0        | 4        | 7       | 0            |
| 2   | S     | 10    | 0        | 4        | 15      | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | E     | 1     | 0        | 0        | 0       | 0            |
| 3   | F     | 1     | 0        | 0        | 0       | 0            |
| 3   | G     | 1     | 0        | 0        | 0       | 0            |
| 3   | I     | 1     | 0        | 0        | 0       | 0            |
| 3   | J     | 2     | 0        | 0        | 0       | 0            |
| 3   | N     | 2     | 0        | 0        | 0       | 0            |
| 3   | O     | 1     | 0        | 0        | 1       | 0            |
| 3   | P     | 1     | 0        | 0        | 0       | 0            |
| 3   | R     | 1     | 0        | 0        | 0       | 0            |
| 3   | S     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 7     | 0        | 0        | 0       | 0            |
| 4   | B     | 2     | 0        | 0        | 0       | 0            |
| 4   | C     | 2     | 0        | 0        | 0       | 0            |
| 4   | D     | 7     | 0        | 0        | 0       | 0            |
| 4   | E     | 5     | 0        | 0        | 0       | 0            |
| 4   | F     | 5     | 0        | 0        | 0       | 0            |
| 4   | G     | 2     | 0        | 0        | 0       | 0            |
| 4   | H     | 2     | 0        | 0        | 0       | 0            |
| 4   | I     | 4     | 0        | 0        | 0       | 0            |
| 4   | J     | 4     | 0        | 0        | 0       | 0            |
| 4   | K     | 8     | 0        | 0        | 0       | 0            |
| 4   | L     | 2     | 0        | 0        | 0       | 0            |
| 4   | M     | 2     | 0        | 0        | 0       | 0            |
| 4   | N     | 2     | 0        | 0        | 0       | 0            |
| 4   | O     | 2     | 0        | 0        | 0       | 0            |
| 4   | P     | 1     | 0        | 0        | 0       | 0            |
| 4   | R     | 3     | 0        | 0        | 0       | 0            |
| 4   | S     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 41248 | 0        | 40450    | 745     | 1            |

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 9.

All (745) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:H:301:MBO:HE6 | 2:H:301:MBO:CE1 | 2.06                     | 1.24              |
| 2:S:301:MBO:HE2 | 2:S:301:MBO:CE3 | 2.06                     | 1.24              |
| 2:B:301:MBO:HE3 | 2:B:301:MBO:CE4 | 2.06                     | 1.24              |
| 2:L:302:MBO:HE6 | 2:L:302:MBO:CE5 | 2.06                     | 1.24              |
| 2:O:301:MBO:HE6 | 2:O:301:MBO:CE1 | 2.06                     | 1.24              |
| 2:R:301:MBO:HE3 | 2:R:301:MBO:CE2 | 2.06                     | 1.24              |
| 2:F:302:MBO:HE3 | 2:F:302:MBO:CE2 | 2.05                     | 1.24              |
| 2:L:301:MBO:HE3 | 2:L:301:MBO:CE2 | 2.06                     | 1.24              |
| 2:S:301:MBO:HE2 | 2:S:301:MBO:CE1 | 2.06                     | 1.24              |
| 2:L:302:MBO:HE6 | 2:L:302:MBO:CE1 | 2.06                     | 1.23              |
| 2:M:301:MBO:HE2 | 2:M:301:MBO:CE1 | 2.06                     | 1.23              |
| 2:D:301:MBO:HE2 | 2:D:301:MBO:CE3 | 2.06                     | 1.23              |
| 2:H:301:MBO:HE6 | 2:H:301:MBO:CE5 | 2.06                     | 1.23              |
| 2:K:301:MBO:HE6 | 2:K:301:MBO:CE5 | 2.06                     | 1.23              |
| 2:P:302:MBO:HE5 | 2:P:302:MBO:CE6 | 2.07                     | 1.23              |
| 2:S:301:MBO:HE3 | 2:S:301:MBO:CE2 | 2.06                     | 1.23              |
| 2:H:301:MBO:HE5 | 2:H:301:MBO:CE4 | 2.06                     | 1.23              |
| 2:H:301:MBO:CE4 | 2:H:301:MBO:HE3 | 2.07                     | 1.23              |
| 2:O:301:MBO:HE6 | 2:O:301:MBO:CE5 | 2.06                     | 1.23              |
| 2:P:302:MBO:HE3 | 2:P:302:MBO:CE2 | 2.06                     | 1.23              |
| 2:B:301:MBO:HE6 | 2:B:301:MBO:CE1 | 2.07                     | 1.23              |
| 2:D:301:MBO:HE5 | 2:D:301:MBO:CE6 | 2.06                     | 1.23              |
| 2:H:301:MBO:HE5 | 2:H:301:MBO:CE6 | 2.06                     | 1.23              |
| 2:H:301:MBO:HE3 | 2:H:301:MBO:CE2 | 2.06                     | 1.23              |
| 2:L:301:MBO:HE6 | 2:L:301:MBO:CE5 | 2.06                     | 1.23              |
| 2:O:301:MBO:HE5 | 2:O:301:MBO:CE4 | 2.06                     | 1.23              |
| 2:R:301:MBO:HE3 | 2:R:301:MBO:CE4 | 2.06                     | 1.23              |
| 2:S:301:MBO:CE1 | 2:S:301:MBO:HE6 | 2.07                     | 1.23              |
| 2:H:302:MBO:HE5 | 2:H:302:MBO:CE4 | 2.07                     | 1.23              |
| 2:I:302:MBO:HE2 | 2:I:302:MBO:CE1 | 2.06                     | 1.23              |
| 2:O:301:MBO:HE5 | 2:O:301:MBO:CE6 | 2.06                     | 1.23              |
| 2:F:302:MBO:HE3 | 2:F:302:MBO:CE4 | 2.06                     | 1.22              |
| 2:K:301:MBO:HE5 | 2:K:301:MBO:CE6 | 2.05                     | 1.22              |
| 2:K:302:MBO:HE3 | 2:K:302:MBO:CE2 | 2.06                     | 1.22              |
| 2:K:302:MBO:HE5 | 2:K:302:MBO:CE6 | 2.06                     | 1.22              |
| 2:M:301:MBO:HE2 | 2:M:301:MBO:CE3 | 2.06                     | 1.22              |
| 2:M:301:MBO:HE5 | 2:M:301:MBO:CE6 | 2.07                     | 1.22              |
| 2:P:302:MBO:HE6 | 2:P:302:MBO:CE1 | 2.06                     | 1.22              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:P:302:MBO:HE6 | 2:P:302:MBO:CE5 | 2.06                     | 1.22              |
| 2:S:301:MBO:HE6 | 2:S:301:MBO:CE5 | 2.07                     | 1.22              |
| 2:F:302:MBO:HE6 | 2:F:302:MBO:CE1 | 2.07                     | 1.22              |
| 2:G:301:MBO:HE3 | 2:G:301:MBO:CE2 | 2.06                     | 1.22              |
| 2:G:301:MBO:HE3 | 2:G:301:MBO:CE4 | 2.07                     | 1.22              |
| 2:H:302:MBO:HE5 | 2:H:302:MBO:CE6 | 2.06                     | 1.22              |
| 2:H:302:MBO:HE3 | 2:H:302:MBO:CE2 | 2.07                     | 1.22              |
| 2:K:302:MBO:HE2 | 2:K:302:MBO:CE3 | 2.06                     | 1.22              |
| 2:L:301:MBO:HE5 | 2:L:301:MBO:CE6 | 2.06                     | 1.22              |
| 2:M:301:MBO:HE3 | 2:M:301:MBO:CE2 | 2.06                     | 1.22              |
| 2:A:302:MBO:HE2 | 2:A:302:MBO:CE3 | 2.06                     | 1.22              |
| 2:C:301:MBO:HE6 | 2:C:301:MBO:CE5 | 2.06                     | 1.22              |
| 2:D:301:MBO:HE6 | 2:D:301:MBO:CE5 | 2.07                     | 1.22              |
| 2:G:301:MBO:HE2 | 2:G:301:MBO:CE3 | 2.07                     | 1.22              |
| 2:L:301:MBO:HE3 | 2:L:301:MBO:CE4 | 2.06                     | 1.22              |
| 2:P:302:MBO:HE3 | 2:P:302:MBO:CE4 | 2.07                     | 1.22              |
| 2:B:301:MBO:HE3 | 2:B:301:MBO:CE2 | 2.06                     | 1.22              |
| 2:C:301:MBO:HE5 | 2:C:301:MBO:CE6 | 2.06                     | 1.22              |
| 2:F:302:MBO:HE5 | 2:F:302:MBO:CE6 | 2.07                     | 1.22              |
| 2:M:301:MBO:HE5 | 2:M:301:MBO:CE4 | 2.07                     | 1.22              |
| 2:C:301:MBO:HE6 | 2:C:301:MBO:CE1 | 2.07                     | 1.22              |
| 2:D:301:MBO:HE2 | 2:D:301:MBO:CE1 | 2.06                     | 1.22              |
| 2:I:302:MBO:HE2 | 2:I:302:MBO:CE3 | 2.06                     | 1.22              |
| 2:M:301:MBO:HE3 | 2:M:301:MBO:CE4 | 2.06                     | 1.22              |
| 2:P:302:MBO:HE5 | 2:P:302:MBO:CE4 | 2.07                     | 1.22              |
| 2:G:301:MBO:HE2 | 2:G:301:MBO:CE1 | 2.06                     | 1.21              |
| 2:K:302:MBO:HE5 | 2:K:302:MBO:CE4 | 2.07                     | 1.21              |
| 2:K:302:MBO:HE2 | 2:K:302:MBO:CE1 | 2.06                     | 1.21              |
| 2:A:302:MBO:HE2 | 2:A:302:MBO:CE1 | 2.06                     | 1.21              |
| 2:A:302:MBO:HE3 | 2:A:302:MBO:CE4 | 2.07                     | 1.21              |
| 2:C:301:MBO:HE5 | 2:C:301:MBO:CE4 | 2.06                     | 1.21              |
| 2:D:301:MBO:HE5 | 2:D:301:MBO:CE4 | 2.07                     | 1.21              |
| 2:F:302:MBO:HE6 | 2:F:302:MBO:CE5 | 2.07                     | 1.21              |
| 2:L:302:MBO:HE2 | 2:L:302:MBO:CE3 | 2.07                     | 1.21              |
| 2:K:301:MBO:HE6 | 2:K:301:MBO:CE1 | 2.06                     | 1.21              |
| 2:K:301:MBO:HE2 | 2:K:301:MBO:CE1 | 2.07                     | 1.21              |
| 2:K:302:MBO:HE3 | 2:K:302:MBO:CE4 | 2.06                     | 1.21              |
| 2:L:301:MBO:HE6 | 2:L:301:MBO:CE1 | 2.06                     | 1.21              |
| 2:A:302:MBO:HE3 | 2:A:302:MBO:CE2 | 2.07                     | 1.21              |
| 2:L:302:MBO:CE1 | 2:L:302:MBO:HE2 | 2.07                     | 1.21              |
| 2:S:301:MBO:HE3 | 2:S:301:MBO:CE4 | 2.06                     | 1.21              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:B:301:MBO:HE6 | 2:B:301:MBO:CE5 | 2.07                     | 1.21              |
| 2:K:301:MBO:HE2 | 2:K:301:MBO:CE3 | 2.07                     | 1.21              |
| 2:L:301:MBO:HE5 | 2:L:301:MBO:CE4 | 2.06                     | 1.21              |
| 2:B:301:MBO:CE4 | 2:B:301:MBO:HE5 | 2.07                     | 1.20              |
| 2:K:301:MBO:HE5 | 2:K:301:MBO:CE4 | 2.06                     | 1.20              |
| 2:B:301:MBO:HE5 | 2:B:301:MBO:CE6 | 2.07                     | 1.20              |
| 2:D:301:MBO:HE6 | 2:D:301:MBO:CE1 | 2.07                     | 1.20              |
| 2:F:302:MBO:CE4 | 2:F:302:MBO:HE5 | 2.08                     | 1.20              |
| 2:H:302:MBO:CE4 | 2:H:302:MBO:HE3 | 2.07                     | 1.19              |
| 2:C:301:MBO:HE6 | 2:C:301:MBO:CE6 | 0.97                     | 1.07              |
| 2:G:301:MBO:CE2 | 2:G:301:MBO:HE2 | 0.97                     | 1.07              |
| 2:K:302:MBO:HE3 | 2:K:302:MBO:CE3 | 0.97                     | 1.07              |
| 2:P:302:MBO:CE6 | 2:P:302:MBO:HE6 | 0.97                     | 1.07              |
| 2:P:302:MBO:HE3 | 2:P:302:MBO:CE3 | 0.97                     | 1.07              |
| 2:S:301:MBO:HE2 | 2:S:301:MBO:CE2 | 0.97                     | 1.07              |
| 2:S:301:MBO:HE6 | 2:S:301:MBO:CE6 | 0.97                     | 1.07              |
| 2:A:302:MBO:HE2 | 2:A:302:MBO:CE2 | 0.97                     | 1.07              |
| 2:A:302:MBO:CE3 | 2:A:302:MBO:HE3 | 0.97                     | 1.07              |
| 2:D:301:MBO:CE6 | 2:D:301:MBO:HE6 | 0.97                     | 1.07              |
| 2:H:302:MBO:HE3 | 2:H:302:MBO:CE3 | 0.97                     | 1.07              |
| 2:L:302:MBO:HE6 | 2:L:302:MBO:CE6 | 0.97                     | 1.07              |
| 2:M:301:MBO:HE5 | 2:M:301:MBO:CE5 | 0.97                     | 1.07              |
| 2:O:301:MBO:CE5 | 2:O:301:MBO:HE5 | 0.97                     | 1.07              |
| 2:P:302:MBO:HE5 | 2:P:302:MBO:CE5 | 0.97                     | 1.07              |
| 2:R:301:MBO:HE3 | 2:R:301:MBO:CE3 | 0.97                     | 1.07              |
| 2:S:301:MBO:CE3 | 2:S:301:MBO:HE3 | 0.97                     | 1.07              |
| 2:B:301:MBO:HE3 | 2:B:301:MBO:CE3 | 0.97                     | 1.06              |
| 2:B:301:MBO:CE5 | 2:B:301:MBO:HE5 | 0.97                     | 1.06              |
| 2:C:301:MBO:CE5 | 2:C:301:MBO:HE5 | 0.97                     | 1.06              |
| 2:H:301:MBO:HE6 | 2:H:301:MBO:CE6 | 0.97                     | 1.06              |
| 2:H:302:MBO:HE5 | 2:H:302:MBO:CE5 | 0.97                     | 1.06              |
| 2:K:302:MBO:CE2 | 2:K:302:MBO:HE2 | 0.97                     | 1.06              |
| 2:K:302:MBO:HE5 | 2:K:302:MBO:CE5 | 0.97                     | 1.06              |
| 2:L:302:MBO:HE2 | 2:L:302:MBO:CE2 | 0.97                     | 1.06              |
| 2:M:301:MBO:HE2 | 2:M:301:MBO:CE2 | 0.97                     | 1.06              |
| 2:M:301:MBO:CE3 | 2:M:301:MBO:HE3 | 0.97                     | 1.06              |
| 2:B:301:MBO:HE6 | 2:B:301:MBO:CE6 | 0.97                     | 1.06              |
| 2:F:302:MBO:HE3 | 2:F:302:MBO:CE3 | 0.97                     | 1.06              |
| 2:F:302:MBO:HE6 | 2:F:302:MBO:CE6 | 0.97                     | 1.06              |
| 2:F:302:MBO:HE5 | 2:F:302:MBO:CE5 | 0.97                     | 1.06              |
| 2:H:301:MBO:CE5 | 2:H:301:MBO:HE5 | 0.97                     | 1.06              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:302:MBO:HE2  | 2:I:302:MBO:CE2  | 0.97                     | 1.06              |
| 2:K:301:MBO:HE6  | 2:K:301:MBO:CE6  | 0.97                     | 1.06              |
| 2:K:301:MBO:HE2  | 2:K:301:MBO:CE2  | 0.97                     | 1.06              |
| 2:L:301:MBO:CE5  | 2:L:301:MBO:HE5  | 0.97                     | 1.06              |
| 2:O:301:MBO:HE6  | 2:O:301:MBO:CE6  | 0.97                     | 1.06              |
| 2:D:301:MBO:HE5  | 2:D:301:MBO:CE5  | 0.97                     | 1.06              |
| 2:G:301:MBO:HE3  | 2:G:301:MBO:CE3  | 0.97                     | 1.06              |
| 2:K:301:MBO:CE5  | 2:K:301:MBO:HE5  | 0.97                     | 1.06              |
| 2:L:301:MBO:HE3  | 2:L:301:MBO:CE3  | 0.97                     | 1.06              |
| 2:L:301:MBO:HE6  | 2:L:301:MBO:CE6  | 0.97                     | 1.06              |
| 2:D:301:MBO:HE2  | 2:D:301:MBO:CE2  | 0.97                     | 1.06              |
| 2:H:301:MBO:HE3  | 2:H:301:MBO:CE3  | 0.97                     | 1.06              |
| 1:F:36:GLN:HE21  | 1:G:103:HIS:CE1  | 1.76                     | 1.02              |
| 1:H:37:LYS:HG3   | 1:H:104:THR:HG22 | 1.45                     | 0.99              |
| 1:F:229:GLN:HA   | 2:F:302:MBO:HE3  | 1.82                     | 0.99              |
| 1:F:36:GLN:HE21  | 1:G:103:HIS:HE1  | 1.02                     | 0.93              |
| 1:A:254:ARG:HH11 | 1:A:254:ARG:HG2  | 1.33                     | 0.91              |
| 1:G:210:ARG:HG3  | 1:G:210:ARG:HH11 | 1.34                     | 0.91              |
| 1:M:230:GLY:HA2  | 2:M:301:MBO:HE2  | 1.91                     | 0.90              |
| 1:L:122:VAL:HG11 | 1:L:155:ILE:HD11 | 1.54                     | 0.90              |
| 2:H:302:MBO:HE5  | 2:H:302:MBO:HE6  | 2.36                     | 0.84              |
| 2:C:301:MBO:HE6  | 2:C:301:MBO:HE5  | 2.37                     | 0.83              |
| 2:H:301:MBO:HE6  | 2:H:301:MBO:HE5  | 2.37                     | 0.83              |
| 2:I:302:MBO:HE2  | 2:I:302:MBO:HE3  | 2.37                     | 0.83              |
| 2:K:301:MBO:HE6  | 2:K:301:MBO:HE5  | 2.37                     | 0.83              |
| 2:L:301:MBO:HE3  | 2:L:301:MBO:HE2  | 2.37                     | 0.83              |
| 2:K:302:MBO:HE3  | 2:K:302:MBO:HE2  | 2.37                     | 0.82              |
| 2:M:301:MBO:HE2  | 2:M:301:MBO:HE3  | 2.36                     | 0.82              |
| 1:R:228:ASP:O    | 2:R:301:MBO:HE3  | 2.17                     | 0.82              |
| 2:P:302:MBO:HE3  | 2:P:302:MBO:HE2  | 2.37                     | 0.82              |
| 1:G:172:HIS:HD2  | 1:G:175:ARG:H    | 1.27                     | 0.82              |
| 2:O:301:MBO:HE6  | 2:O:301:MBO:HE5  | 2.36                     | 0.82              |
| 1:M:172:HIS:HD2  | 1:M:175:ARG:H    | 1.26                     | 0.82              |
| 2:S:301:MBO:HE2  | 2:S:301:MBO:HE3  | 2.37                     | 0.82              |
| 2:F:302:MBO:HE3  | 2:F:302:MBO:HE2  | 2.36                     | 0.82              |
| 2:L:301:MBO:HE6  | 2:L:301:MBO:HE5  | 2.37                     | 0.82              |
| 2:R:301:MBO:HE3  | 2:R:301:MBO:HE2  | 2.36                     | 0.82              |
| 2:A:302:MBO:HE2  | 2:A:302:MBO:HE3  | 2.37                     | 0.81              |
| 2:H:301:MBO:HE3  | 2:H:301:MBO:HE2  | 2.38                     | 0.81              |
| 2:L:302:MBO:HE2  | 2:L:302:MBO:HE3  | 2.37                     | 0.81              |
| 2:M:301:MBO:HE5  | 2:M:301:MBO:HE6  | 2.37                     | 0.81              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:P:302:MBO:HE5 | 2:P:302:MBO:HE6  | 2.37                     | 0.81              |
| 2:D:301:MBO:HE2 | 2:D:301:MBO:HE3  | 2.37                     | 0.81              |
| 2:G:301:MBO:HE3 | 2:G:301:MBO:HE2  | 2.38                     | 0.81              |
| 1:N:13:GLU:HG3  | 1:N:154:LYS:HE2  | 1.62                     | 0.81              |
| 2:B:301:MBO:HE3 | 2:B:301:MBO:HE2  | 2.36                     | 0.81              |
| 2:B:301:MBO:HE6 | 2:B:301:MBO:HE5  | 2.38                     | 0.81              |
| 2:D:301:MBO:HE5 | 2:D:301:MBO:HE6  | 2.38                     | 0.81              |
| 2:L:302:MBO:HE6 | 2:L:302:MBO:HE5  | 2.37                     | 0.81              |
| 1:P:230:GLY:HA2 | 2:P:302:MBO:HE2  | 2.01                     | 0.81              |
| 2:F:302:MBO:HE6 | 2:F:302:MBO:HE5  | 2.39                     | 0.80              |
| 1:R:172:HIS:HD2 | 1:R:175:ARG:H    | 1.28                     | 0.79              |
| 2:S:301:MBO:HE6 | 2:S:301:MBO:HE5  | 2.38                     | 0.79              |
| 2:K:302:MBO:HE5 | 2:K:302:MBO:HE6  | 2.37                     | 0.79              |
| 1:E:188:PRO:HA  | 1:E:217:MET:HE1  | 1.64                     | 0.79              |
| 1:H:37:LYS:HG3  | 1:H:104:THR:CG2  | 2.14                     | 0.77              |
| 2:H:302:MBO:HE3 | 2:H:302:MBO:HE2  | 2.39                     | 0.77              |
| 1:M:90:MET:HB3  | 1:N:49:SER:HB2   | 1.66                     | 0.77              |
| 2:K:301:MBO:HE2 | 2:K:301:MBO:HE3  | 2.39                     | 0.76              |
| 1:N:115:ARG:HD2 | 1:N:134:ASP:OD2  | 1.84                     | 0.76              |
| 1:E:228:ASP:O   | 2:E:301:MBO:HE3  | 2.23                     | 0.76              |
| 1:G:115:ARG:HG3 | 1:G:115:ARG:HH11 | 1.48                     | 0.76              |
| 1:B:25:VAL:HG22 | 1:B:114:THR:HG22 | 1.69                     | 0.75              |
| 1:I:228:ASP:O   | 2:I:302:MBO:HE5  | 2.26                     | 0.74              |
| 1:C:36:GLN:HG3  | 1:D:103:HIS:CE1  | 2.23                     | 0.73              |
| 1:L:122:VAL:CG1 | 1:L:155:ILE:HD11 | 2.19                     | 0.73              |
| 1:L:283:CYS:SG  | 2:L:301:MBO:HG   | 2.07                     | 0.72              |
| 1:F:229:GLN:CA  | 2:F:302:MBO:HE3  | 2.56                     | 0.72              |
| 1:K:67:GLY:O    | 1:K:69:ALA:N     | 2.22                     | 0.72              |
| 1:M:73:GLY:HA2  | 1:N:67:GLY:H     | 1.53                     | 0.72              |
| 1:M:230:GLY:CA  | 2:M:301:MBO:HE2  | 2.58                     | 0.72              |
| 1:H:266:PHE:CD1 | 2:H:302:MBO:HE6  | 2.62                     | 0.71              |
| 1:S:228:ASP:O   | 2:S:301:MBO:HE3  | 2.29                     | 0.71              |
| 1:M:14:VAL:HG21 | 1:M:123:GLY:O    | 1.90                     | 0.71              |
| 1:L:90:MET:HB3  | 1:M:49:SER:HB2   | 1.70                     | 0.70              |
| 1:M:266:PHE:HB3 | 2:M:301:MBO:HE6  | 2.10                     | 0.70              |
| 1:H:20:TRP:HZ3  | 1:H:116:TRP:CE3  | 2.10                     | 0.70              |
| 1:S:192:LEU:HB2 | 1:S:280:ASN:HD21 | 1.56                     | 0.70              |
| 1:S:283:CYS:SG  | 2:S:301:MBO:HG   | 2.10                     | 0.69              |
| 1:G:29:ARG:HB2  | 1:H:135:GLU:HB3  | 1.76                     | 0.68              |
| 1:P:230:GLY:CA  | 2:P:302:MBO:HE2  | 2.61                     | 0.68              |
| 1:E:9:TYR:HE2   | 1:E:11:GLN:HE21  | 1.41                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:188:PRO:HD3  | 1:I:218:TYR:HD1  | 1.58                     | 0.68              |
| 1:F:230:GLY:HA2  | 2:F:302:MBO:HE2  | 2.13                     | 0.68              |
| 1:J:117:GLN:HG3  | 1:J:132:LEU:HD13 | 1.76                     | 0.68              |
| 1:D:36:GLN:HG3   | 1:E:103:HIS:NE2  | 2.08                     | 0.68              |
| 2:O:301:MBO:HE5  | 2:O:301:MBO:CZ   | 2.61                     | 0.68              |
| 1:G:172:HIS:CD2  | 1:G:175:ARG:H    | 2.12                     | 0.67              |
| 2:B:301:MBO:HE3  | 2:B:301:MBO:CZ   | 2.63                     | 0.67              |
| 1:P:90:MET:HB3   | 1:R:49:SER:HB2   | 1.74                     | 0.67              |
| 1:R:55:THR:HB    | 1:R:86:SER:HB2   | 1.75                     | 0.67              |
| 2:H:302:MBO:HE5  | 2:H:302:MBO:CZ   | 2.63                     | 0.67              |
| 2:R:301:MBO:HE3  | 2:R:301:MBO:CZ   | 2.63                     | 0.67              |
| 2:F:302:MBO:HE3  | 2:F:302:MBO:CZ   | 2.62                     | 0.66              |
| 1:J:76:GLU:O     | 1:K:62:SER:HB2   | 1.96                     | 0.66              |
| 1:N:84:GLN:HB3   | 1:O:55:THR:HG23  | 1.77                     | 0.66              |
| 1:J:155:ILE:HG22 | 1:K:145:ILE:HB   | 1.76                     | 0.66              |
| 2:K:301:MBO:HE5  | 2:K:301:MBO:CZ   | 2.63                     | 0.66              |
| 1:N:100:VAL:HB   | 1:O:39:THR:HG23  | 1.77                     | 0.66              |
| 2:A:302:MBO:HE3  | 2:A:302:MBO:CZ   | 2.64                     | 0.66              |
| 1:P:41:THR:HG23  | 1:P:100:VAL:HG22 | 1.76                     | 0.66              |
| 1:D:115:ARG:HD2  | 1:D:134:ASP:OD2  | 1.95                     | 0.66              |
| 1:L:282:TYR:HB3  | 1:L:284:LEU:CD2  | 2.26                     | 0.66              |
| 2:M:301:MBO:HE3  | 2:M:301:MBO:CZ   | 2.64                     | 0.66              |
| 1:M:41:THR:HG23  | 1:M:100:VAL:HG22 | 1.78                     | 0.66              |
| 1:O:100:VAL:HB   | 1:P:39:THR:HG23  | 1.78                     | 0.66              |
| 1:O:103:HIS:NE2  | 1:P:36:GLN:HG3   | 2.11                     | 0.65              |
| 1:R:39:THR:HB    | 1:R:102:GLU:HG3  | 1.77                     | 0.65              |
| 2:S:301:MBO:HE3  | 2:S:301:MBO:CZ   | 2.65                     | 0.65              |
| 1:C:115:ARG:HD3  | 1:C:134:ASP:OD2  | 1.96                     | 0.65              |
| 1:E:51:THR:HB    | 1:F:88:VAL:HG13  | 1.78                     | 0.65              |
| 1:K:228:ASP:O    | 2:K:301:MBO:HE5  | 2.35                     | 0.65              |
| 1:D:283:CYS:SG   | 2:D:301:MBO:HG   | 2.15                     | 0.65              |
| 1:O:232:ILE:HD11 | 1:O:283:CYS:HB2  | 1.78                     | 0.64              |
| 1:O:269:SER:HB3  | 2:O:301:MBO:HE6  | 2.17                     | 0.64              |
| 1:G:248:ASN:HB3  | 1:G:260:THR:HG22 | 1.79                     | 0.64              |
| 1:J:64:ILE:HG13  | 1:S:75:VAL:HG22  | 1.79                     | 0.64              |
| 1:R:17:VAL:HG13  | 1:R:150:THR:HG22 | 1.78                     | 0.64              |
| 1:R:115:ARG:HD3  | 1:R:134:ASP:OD2  | 1.97                     | 0.64              |
| 2:H:301:MBO:HE5  | 2:H:301:MBO:CZ   | 2.65                     | 0.64              |
| 1:P:84:GLN:HB3   | 1:R:55:THR:HG23  | 1.79                     | 0.64              |
| 1:G:172:HIS:HE1  | 1:G:289:ASP:OD2  | 1.78                     | 0.64              |
| 1:F:14:VAL:HG12  | 1:F:155:ILE:HD13 | 1.79                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:301:MBO:HE5  | 2:C:301:MBO:CZ   | 2.66                     | 0.64              |
| 1:O:25:VAL:HG22  | 1:O:114:THR:HG22 | 1.80                     | 0.64              |
| 1:G:67:GLY:O     | 1:G:69:ALA:N     | 2.31                     | 0.63              |
| 1:B:53:THR:HG23  | 1:B:88:VAL:HG22  | 1.79                     | 0.63              |
| 1:D:55:THR:HG23  | 1:E:84:GLN:HB3   | 1.78                     | 0.63              |
| 1:F:36:GLN:NE2   | 1:G:103:HIS:HE1  | 1.85                     | 0.63              |
| 1:O:272:CYS:SG   | 3:O:302:HG:HG    | 2.16                     | 0.63              |
| 1:G:283:CYS:SG   | 2:G:301:MBO:HG   | 2.17                     | 0.63              |
| 1:K:84:GLN:HB3   | 1:L:55:THR:HG23  | 1.80                     | 0.63              |
| 2:K:302:MBO:HE5  | 2:K:302:MBO:CZ   | 2.67                     | 0.63              |
| 1:N:14:VAL:HG21  | 1:N:123:GLY:O    | 1.98                     | 0.63              |
| 1:B:269:SER:HB3  | 2:B:302:MBO:HE6  | 2.19                     | 0.62              |
| 2:K:302:MBO:HE3  | 2:K:302:MBO:CZ   | 2.67                     | 0.62              |
| 1:O:269:SER:CB   | 2:O:301:MBO:HE6  | 2.68                     | 0.62              |
| 1:P:33:SER:HB3   | 1:P:109:PRO:HD3  | 1.81                     | 0.62              |
| 1:C:49:SER:HB2   | 1:D:90:MET:HG2   | 1.81                     | 0.62              |
| 1:K:103:HIS:NE2  | 1:L:36:GLN:HG3   | 2.15                     | 0.62              |
| 1:C:39:THR:HG23  | 1:D:100:VAL:HB   | 1.82                     | 0.61              |
| 1:D:228:ASP:O    | 2:D:301:MBO:HE3  | 2.38                     | 0.61              |
| 1:H:266:PHE:CE1  | 2:H:302:MBO:HE6  | 2.73                     | 0.61              |
| 1:H:20:TRP:CZ3   | 1:H:116:TRP:CE3  | 2.89                     | 0.61              |
| 1:N:45:LYS:HG3   | 1:N:96:TYR:HB3   | 1.81                     | 0.61              |
| 2:L:301:MBO:HE3  | 2:L:301:MBO:CZ   | 2.67                     | 0.61              |
| 2:P:302:MBO:HE3  | 2:P:302:MBO:CZ   | 2.68                     | 0.61              |
| 1:H:40:ILE:HG13  | 1:H:101:ILE:HG23 | 1.80                     | 0.61              |
| 1:K:225:TYR:CD1  | 1:K:235:ASP:HB2  | 2.36                     | 0.61              |
| 1:M:100:VAL:HB   | 1:N:39:THR:HG23  | 1.82                     | 0.61              |
| 1:S:14:VAL:HG22  | 1:S:155:ILE:CD1  | 2.31                     | 0.61              |
| 1:K:100:VAL:HB   | 1:L:39:THR:HG23  | 1.82                     | 0.61              |
| 1:L:41:THR:HG23  | 1:L:100:VAL:HG22 | 1.82                     | 0.61              |
| 1:S:269:SER:HB3  | 2:S:301:MBO:HE6  | 2.21                     | 0.61              |
| 1:I:20:TRP:HZ3   | 1:I:116:TRP:CE3  | 2.19                     | 0.60              |
| 1:R:90:MET:HG2   | 1:S:49:SER:HB3   | 1.81                     | 0.60              |
| 1:M:287:ARG:HH11 | 2:M:302:MBO:HE6  | 2.05                     | 0.60              |
| 1:P:34:VAL:HG23  | 1:P:107:ILE:HB   | 1.83                     | 0.60              |
| 2:D:301:MBO:HE5  | 2:D:301:MBO:CZ   | 2.67                     | 0.60              |
| 2:P:302:MBO:HE5  | 2:P:302:MBO:CZ   | 2.70                     | 0.60              |
| 1:H:225:TYR:CD1  | 1:H:235:ASP:HB2  | 2.35                     | 0.60              |
| 2:G:301:MBO:HE3  | 2:G:301:MBO:CZ   | 2.70                     | 0.60              |
| 1:C:59:SER:HB2   | 1:D:80:SER:HB3   | 1.83                     | 0.60              |
| 1:A:109:PRO:O    | 1:A:110:THR:HB   | 2.02                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:238:THR:O    | 1:R:244:ARG:NH2  | 2.35                     | 0.60              |
| 1:L:53:THR:HG23  | 1:L:88:VAL:HG22  | 1.82                     | 0.59              |
| 2:H:301:MBO:HE3  | 2:H:301:MBO:CZ   | 2.70                     | 0.59              |
| 1:O:67:GLY:O     | 1:O:69:ALA:N     | 2.32                     | 0.59              |
| 1:J:188:PRO:HD3  | 1:J:218:TYR:HD1  | 1.68                     | 0.59              |
| 2:M:301:MBO:HE5  | 2:M:301:MBO:CZ   | 2.71                     | 0.59              |
| 1:J:20:TRP:HB2   | 1:J:147:GLN:HA   | 1.85                     | 0.59              |
| 2:L:301:MBO:HE5  | 2:L:301:MBO:CZ   | 2.69                     | 0.59              |
| 1:R:172:HIS:CD2  | 1:R:175:ARG:H    | 2.15                     | 0.59              |
| 1:M:75:VAL:HG22  | 1:N:64:ILE:HG12  | 1.85                     | 0.58              |
| 1:R:84:GLN:HB3   | 1:S:55:THR:HG23  | 1.84                     | 0.58              |
| 2:H:302:MBO:HE3  | 2:H:302:MBO:CZ   | 2.71                     | 0.58              |
| 1:K:122:VAL:CG1  | 1:K:155:ILE:HD11 | 2.33                     | 0.58              |
| 1:R:90:MET:HG2   | 1:S:49:SER:CB    | 2.34                     | 0.58              |
| 1:M:25:VAL:HG22  | 1:M:114:THR:HG22 | 1.85                     | 0.58              |
| 1:H:25:VAL:HG22  | 1:H:114:THR:HG22 | 1.84                     | 0.58              |
| 1:O:269:SER:OG   | 2:O:301:MBO:HE6  | 2.41                     | 0.58              |
| 1:E:53:THR:HB    | 1:F:86:SER:HB3   | 1.85                     | 0.58              |
| 1:N:122:VAL:HG11 | 1:N:155:ILE:HD11 | 1.84                     | 0.58              |
| 1:A:269:SER:HB3  | 2:A:301:MBO:HE6  | 2.24                     | 0.57              |
| 1:L:282:TYR:HB3  | 1:L:284:LEU:HD22 | 1.85                     | 0.57              |
| 1:P:230:GLY:N    | 2:P:302:MBO:HE2  | 2.57                     | 0.57              |
| 1:B:268:ARG:HD2  | 1:C:278:ALA:HB1  | 1.85                     | 0.57              |
| 1:H:284:LEU:CD1  | 2:H:301:MBO:HE6  | 2.72                     | 0.57              |
| 1:K:53:THR:HG23  | 1:K:88:VAL:HG22  | 1.86                     | 0.57              |
| 1:S:39:THR:HB    | 1:S:102:GLU:HG3  | 1.87                     | 0.57              |
| 1:G:210:ARG:HG3  | 1:G:210:ARG:NH1  | 2.11                     | 0.57              |
| 1:F:33:SER:HB3   | 1:F:109:PRO:HD3  | 1.86                     | 0.57              |
| 1:O:41:THR:HG23  | 1:O:100:VAL:HG22 | 1.86                     | 0.57              |
| 1:E:33:SER:HB3   | 1:E:109:PRO:HD3  | 1.87                     | 0.56              |
| 1:M:42:LYS:HE3   | 1:M:130:MET:HE1  | 1.86                     | 0.56              |
| 1:H:172:HIS:HD2  | 1:H:175:ARG:H    | 1.52                     | 0.56              |
| 1:M:115:ARG:HD3  | 1:M:134:ASP:OD2  | 2.06                     | 0.56              |
| 1:D:49:SER:HB3   | 1:D:92:GLN:HG3   | 1.86                     | 0.56              |
| 1:G:36:GLN:NE2   | 1:H:103:HIS:NE2  | 2.48                     | 0.56              |
| 1:J:14:VAL:HG21  | 1:J:123:GLY:O    | 2.05                     | 0.56              |
| 1:G:49:SER:HB2   | 1:H:90:MET:HB2   | 1.88                     | 0.56              |
| 1:H:40:ILE:HG13  | 1:H:101:ILE:CG2  | 2.36                     | 0.56              |
| 1:L:100:VAL:HB   | 1:M:39:THR:HG23  | 1.88                     | 0.56              |
| 1:B:49:SER:HB3   | 1:B:92:GLN:HG3   | 1.88                     | 0.56              |
| 2:F:302:MBO:HE5  | 2:F:302:MBO:CZ   | 2.73                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:255:HIS:HB2  | 1:H:295:VAL:CG2  | 2.36                     | 0.56              |
| 1:M:47:VAL:HG22  | 1:M:94:GLU:HB3   | 1.88                     | 0.56              |
| 1:S:14:VAL:HG22  | 1:S:155:ILE:HD11 | 1.88                     | 0.56              |
| 1:F:266:PHE:HB2  | 1:F:269:SER:OG   | 2.06                     | 0.56              |
| 1:I:157:VAL:HB   | 1:I:254:ARG:HD3  | 1.88                     | 0.56              |
| 1:L:25:VAL:HG22  | 1:L:114:THR:HG22 | 1.86                     | 0.56              |
| 1:E:188:PRO:HB2  | 1:E:234:PHE:HB2  | 1.87                     | 0.55              |
| 1:I:13:GLU:HG2   | 1:I:154:LYS:HG3  | 1.87                     | 0.55              |
| 1:N:53:THR:HG23  | 1:N:88:VAL:HG22  | 1.88                     | 0.55              |
| 1:P:225:TYR:CD1  | 1:P:235:ASP:HB2  | 2.40                     | 0.55              |
| 1:L:228:ASP:O    | 2:L:301:MBO:HE5  | 2.43                     | 0.55              |
| 1:S:53:THR:HG23  | 1:S:88:VAL:HG22  | 1.87                     | 0.55              |
| 1:K:236:GLN:O    | 1:K:243:GLN:NE2  | 2.39                     | 0.55              |
| 1:L:195:SER:OG   | 1:L:197:LEU:HD12 | 2.06                     | 0.55              |
| 1:C:99:LYS:HE3   | 1:C:101:ILE:HD11 | 1.87                     | 0.55              |
| 1:P:266:PHE:HB3  | 2:P:302:MBO:HE6  | 2.26                     | 0.55              |
| 1:E:145:ILE:HB   | 1:F:155:ILE:HG13 | 1.88                     | 0.55              |
| 1:A:268:ARG:HD2  | 1:B:278:ALA:HB1  | 1.88                     | 0.55              |
| 1:H:284:LEU:HA   | 2:H:302:MBO:HE2  | 2.27                     | 0.55              |
| 1:J:162:ILE:HG23 | 1:J:165:LYS:HB3  | 1.87                     | 0.55              |
| 1:L:73:GLY:HA2   | 1:M:67:GLY:H     | 1.71                     | 0.55              |
| 1:N:48:ASN:HB2   | 1:N:93:THR:HG22  | 1.88                     | 0.55              |
| 2:B:301:MBO:HE5  | 2:B:301:MBO:CZ   | 2.72                     | 0.55              |
| 1:I:184:ARG:HD2  | 1:I:278:ALA:HB3  | 1.89                     | 0.55              |
| 1:B:188:PRO:HB2  | 1:B:234:PHE:HB2  | 1.89                     | 0.54              |
| 1:H:147:GLN:HB2  | 1:I:155:ILE:HD12 | 1.88                     | 0.54              |
| 1:I:188:PRO:HD3  | 1:I:218:TYR:CD1  | 2.42                     | 0.54              |
| 1:B:41:THR:HG23  | 1:B:100:VAL:HG22 | 1.88                     | 0.54              |
| 1:B:39:THR:HG23  | 1:C:100:VAL:HB   | 1.89                     | 0.54              |
| 1:G:248:ASN:HB3  | 1:G:260:THR:CG2  | 2.36                     | 0.54              |
| 1:H:266:PHE:CG   | 2:H:302:MBO:HE6  | 2.80                     | 0.54              |
| 1:K:116:TRP:HH2  | 1:K:143:GLN:NE2  | 2.04                     | 0.54              |
| 1:K:269:SER:HB3  | 2:K:301:MBO:HE2  | 2.27                     | 0.54              |
| 1:A:162:ILE:HG23 | 1:A:165:LYS:HB3  | 1.88                     | 0.54              |
| 1:C:55:THR:HG23  | 1:D:84:GLN:HB3   | 1.88                     | 0.54              |
| 1:S:115:ARG:HD3  | 1:S:134:ASP:OD2  | 2.07                     | 0.54              |
| 1:A:254:ARG:HG2  | 1:A:254:ARG:NH1  | 2.11                     | 0.54              |
| 1:C:282:TYR:HB3  | 1:C:284:LEU:HD23 | 1.88                     | 0.54              |
| 1:M:14:VAL:HG11  | 1:M:155:ILE:HD11 | 1.89                     | 0.54              |
| 1:A:20:TRP:HA    | 1:A:118:LEU:HG   | 1.90                     | 0.54              |
| 1:A:84:GLN:HB3   | 1:I:55:THR:HG23  | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:230:GLY:N    | 2:F:302:MBO:HE2  | 2.61                     | 0.54              |
| 1:P:18:ALA:HB1   | 1:P:118:LEU:HD12 | 1.90                     | 0.54              |
| 1:N:75:VAL:HG22  | 1:O:64:ILE:HD12  | 1.89                     | 0.54              |
| 1:I:160:GLN:NE2  | 1:I:252:PRO:HB3  | 2.22                     | 0.54              |
| 1:A:110:THR:O    | 1:A:110:THR:CG2  | 2.56                     | 0.54              |
| 1:M:84:GLN:HB3   | 1:N:55:THR:HG23  | 1.90                     | 0.54              |
| 1:A:33:SER:HB3   | 1:A:109:PRO:HD3  | 1.90                     | 0.53              |
| 1:D:99:LYS:HE3   | 1:D:101:ILE:HD11 | 1.89                     | 0.53              |
| 1:F:228:ASP:O    | 2:F:302:MBO:HE3  | 2.46                     | 0.53              |
| 1:I:203:TYR:HE1  | 1:I:212:LYS:HD3  | 1.74                     | 0.53              |
| 1:J:192:LEU:HD13 | 1:J:281:VAL:HG22 | 1.91                     | 0.53              |
| 1:G:20:TRP:HB2   | 1:G:147:GLN:HA   | 1.89                     | 0.53              |
| 1:O:20:TRP:HB2   | 1:O:147:GLN:HA   | 1.90                     | 0.53              |
| 1:S:25:VAL:HG22  | 1:S:114:THR:HG22 | 1.89                     | 0.53              |
| 1:G:14:VAL:HG22  | 1:G:155:ILE:HD11 | 1.90                     | 0.53              |
| 1:K:99:LYS:HE3   | 1:K:101:ILE:HD11 | 1.90                     | 0.53              |
| 1:B:205:ASP:OD1  | 1:B:244:ARG:NH1  | 2.41                     | 0.53              |
| 1:C:260:THR:HG22 | 1:C:290:LYS:HA   | 1.90                     | 0.53              |
| 1:L:99:LYS:HE2   | 1:L:101:ILE:HD11 | 1.91                     | 0.53              |
| 1:M:266:PHE:CB   | 2:M:301:MBO:HE6  | 2.77                     | 0.53              |
| 1:H:247:ILE:HG23 | 1:H:249:LYS:H    | 1.74                     | 0.53              |
| 1:K:249:LYS:HE3  | 1:K:253:LEU:HD23 | 1.90                     | 0.53              |
| 1:G:49:SER:HB2   | 1:H:90:MET:CB    | 2.39                     | 0.53              |
| 1:R:19:VAL:HG22  | 1:R:148:VAL:HG22 | 1.89                     | 0.53              |
| 1:L:115:ARG:HD2  | 1:L:132:LEU:HD22 | 1.91                     | 0.53              |
| 1:M:94:GLU:HG3   | 1:N:45:LYS:HB3   | 1.91                     | 0.53              |
| 1:D:146:PRO:CB   | 1:D:149:ILE:HD11 | 2.38                     | 0.52              |
| 1:M:246:ALA:HB2  | 1:M:264:LYS:HE2  | 1.91                     | 0.52              |
| 1:N:184:ARG:HG2  | 1:N:185:LYS:HD2  | 1.91                     | 0.52              |
| 1:F:109:PRO:HG2  | 1:L:109:PRO:HG2  | 1.92                     | 0.52              |
| 1:H:163:LEU:HD11 | 1:H:251:LEU:HD21 | 1.91                     | 0.52              |
| 1:G:47:VAL:HA    | 1:G:93:THR:O     | 2.08                     | 0.52              |
| 1:N:72:ILE:HG12  | 1:O:69:ALA:HB2   | 1.91                     | 0.52              |
| 1:O:269:SER:HG   | 2:O:301:MBO:HE6  | 2.12                     | 0.52              |
| 1:D:14:VAL:HG12  | 1:D:155:ILE:HD13 | 1.91                     | 0.52              |
| 1:K:13:GLU:HG2   | 1:K:152:ARG:HH21 | 1.75                     | 0.52              |
| 1:P:47:VAL:HG22  | 1:P:94:GLU:HG2   | 1.91                     | 0.52              |
| 1:G:159:ARG:CB   | 1:G:159:ARG:HH11 | 2.22                     | 0.52              |
| 1:L:47:VAL:HG22  | 1:L:94:GLU:HG3   | 1.92                     | 0.52              |
| 1:H:25:VAL:HG22  | 1:H:114:THR:CG2  | 2.40                     | 0.52              |
| 1:H:33:SER:HB3   | 1:H:109:PRO:HD3  | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:230:GLY:CA   | 2:F:302:MBO:HE2  | 2.78                     | 0.52              |
| 1:G:29:ARG:HB2   | 1:H:135:GLU:CB   | 2.39                     | 0.51              |
| 1:I:20:TRP:CZ3   | 1:I:116:TRP:CE3  | 2.99                     | 0.51              |
| 1:N:105:ILE:HB   | 1:O:34:VAL:HG12  | 1.91                     | 0.51              |
| 1:N:172:HIS:HD2  | 1:N:175:ARG:H    | 1.57                     | 0.51              |
| 1:A:20:TRP:HB2   | 1:A:147:GLN:HA   | 1.93                     | 0.51              |
| 1:G:59:SER:HB2   | 1:H:80:SER:HB3   | 1.93                     | 0.51              |
| 1:G:192:LEU:HD22 | 1:G:273:TYR:CD1  | 2.46                     | 0.51              |
| 1:H:146:PRO:HB2  | 1:H:149:ILE:HD11 | 1.92                     | 0.51              |
| 1:I:164:GLY:HA2  | 1:I:203:TYR:CE2  | 2.46                     | 0.51              |
| 1:J:102:GLU:O    | 1:K:36:GLN:HA    | 2.10                     | 0.51              |
| 1:N:122:VAL:CG1  | 1:N:155:ILE:HD11 | 2.41                     | 0.51              |
| 1:O:14:VAL:HG21  | 1:O:123:GLY:O    | 2.11                     | 0.51              |
| 1:A:86:SER:HB3   | 1:I:53:THR:HB    | 1.92                     | 0.51              |
| 1:R:157:VAL:HB   | 1:R:254:ARG:HD3  | 1.92                     | 0.51              |
| 1:S:190:ALA:HB3  | 1:S:232:ILE:HG22 | 1.93                     | 0.51              |
| 1:B:232:ILE:HD11 | 1:B:283:CYS:HB2  | 1.92                     | 0.51              |
| 1:M:31:SER:HA    | 1:M:109:PRO:HB3  | 1.93                     | 0.51              |
| 1:M:184:ARG:HG2  | 1:M:185:LYS:HD2  | 1.93                     | 0.51              |
| 1:S:41:THR:HG23  | 1:S:100:VAL:HG22 | 1.93                     | 0.51              |
| 1:C:14:VAL:HG21  | 1:C:123:GLY:O    | 2.11                     | 0.51              |
| 1:S:210:ARG:HG2  | 1:S:223:TYR:CD2  | 2.46                     | 0.51              |
| 1:C:31:SER:HA    | 1:C:109:PRO:HB3  | 1.92                     | 0.51              |
| 1:G:227:SER:C    | 1:G:229:GLN:H    | 2.17                     | 0.51              |
| 1:H:20:TRP:CD1   | 1:H:20:TRP:C     | 2.88                     | 0.51              |
| 1:N:172:HIS:CD2  | 1:N:175:ARG:H    | 2.28                     | 0.51              |
| 1:A:67:GLY:C     | 1:A:69:ALA:H     | 2.18                     | 0.50              |
| 1:A:188:PRO:HG2  | 1:A:234:PHE:HB2  | 1.93                     | 0.50              |
| 1:G:53:THR:HG23  | 1:G:88:VAL:HB    | 1.93                     | 0.50              |
| 1:H:284:LEU:HD12 | 2:H:301:MBO:HE6  | 2.31                     | 0.50              |
| 1:B:36:GLN:HG3   | 1:C:103:HIS:NE2  | 2.26                     | 0.50              |
| 1:C:39:THR:HB    | 1:C:102:GLU:HG3  | 1.93                     | 0.50              |
| 1:H:184:ARG:HD2  | 1:H:278:ALA:HB3  | 1.94                     | 0.50              |
| 1:I:14:VAL:HG21  | 1:I:123:GLY:O    | 2.11                     | 0.50              |
| 1:E:99:LYS:HE2   | 1:E:101:ILE:HD11 | 1.94                     | 0.50              |
| 1:P:86:SER:HB3   | 1:R:53:THR:HB    | 1.94                     | 0.50              |
| 1:P:180:THR:HG23 | 1:P:198:PHE:CE1  | 2.46                     | 0.50              |
| 1:B:39:THR:HB    | 1:B:102:GLU:HG3  | 1.93                     | 0.50              |
| 1:C:269:SER:HG   | 2:C:301:MBO:HE6  | 2.15                     | 0.50              |
| 1:E:269:SER:HB3  | 2:E:301:MBO:HE6  | 2.32                     | 0.50              |
| 1:I:225:TYR:CD1  | 1:I:235:ASP:HB2  | 2.47                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:260:THR:HG22 | 1:O:290:LYS:HA   | 1.94                     | 0.50              |
| 1:K:45:LYS:O     | 1:K:46:ASN:ND2   | 2.41                     | 0.50              |
| 1:D:210:ARG:HG2  | 1:D:243:GLN:O    | 2.12                     | 0.50              |
| 1:D:248:ASN:HB3  | 1:D:260:THR:CG2  | 2.42                     | 0.50              |
| 1:E:269:SER:HG   | 2:E:301:MBO:HE6  | 2.14                     | 0.50              |
| 1:O:84:GLN:HB3   | 1:P:55:THR:HG23  | 1.94                     | 0.50              |
| 1:D:269:SER:HB3  | 2:D:301:MBO:HE6  | 2.32                     | 0.49              |
| 1:F:36:GLN:NE2   | 1:G:103:HIS:CE1  | 2.62                     | 0.49              |
| 1:H:146:PRO:CB   | 1:H:149:ILE:HD11 | 2.43                     | 0.49              |
| 1:P:75:VAL:HG22  | 1:R:64:ILE:HG12  | 1.95                     | 0.49              |
| 1:D:175:ARG:NH1  | 1:D:177:GLU:OE1  | 2.45                     | 0.49              |
| 1:L:57:THR:HG23  | 1:L:84:GLN:HB3   | 1.92                     | 0.49              |
| 1:M:115:ARG:CD   | 1:M:134:ASP:OD2  | 2.60                     | 0.49              |
| 1:O:17:VAL:HG22  | 1:O:150:THR:HG22 | 1.94                     | 0.49              |
| 1:S:47:VAL:HG22  | 1:S:94:GLU:HG3   | 1.94                     | 0.49              |
| 1:D:41:THR:HG23  | 1:D:100:VAL:HG22 | 1.93                     | 0.49              |
| 1:O:39:THR:HB    | 1:O:102:GLU:HG3  | 1.93                     | 0.49              |
| 1:J:84:GLN:HB3   | 1:K:55:THR:HG23  | 1.95                     | 0.49              |
| 1:A:254:ARG:HH11 | 1:A:254:ARG:CG   | 2.15                     | 0.49              |
| 1:N:76:GLU:O     | 1:O:62:SER:HB2   | 2.13                     | 0.49              |
| 1:B:31:SER:O     | 1:R:109:PRO:HG2  | 2.13                     | 0.49              |
| 1:S:164:GLY:HA2  | 1:S:203:TYR:CE2  | 2.48                     | 0.49              |
| 1:D:37:LYS:HB3   | 1:E:102:GLU:HG2  | 1.94                     | 0.48              |
| 1:M:20:TRP:HB2   | 1:M:147:GLN:HA   | 1.95                     | 0.48              |
| 1:R:90:MET:CG    | 1:S:49:SER:HB3   | 2.43                     | 0.48              |
| 1:O:17:VAL:HG13  | 1:O:150:THR:HG22 | 1.94                     | 0.48              |
| 1:P:241:PRO:HB2  | 1:P:265:TYR:HB2  | 1.95                     | 0.48              |
| 1:A:117:GLN:HG3  | 1:A:132:LEU:HD21 | 1.94                     | 0.48              |
| 1:I:20:TRP:CD1   | 1:I:20:TRP:C     | 2.92                     | 0.48              |
| 1:J:36:GLN:HG3   | 1:S:103:HIS:NE2  | 2.29                     | 0.48              |
| 1:G:37:LYS:HB3   | 1:H:102:GLU:HG2  | 1.96                     | 0.48              |
| 1:L:20:TRP:HB2   | 1:L:147:GLN:HA   | 1.95                     | 0.48              |
| 1:M:260:THR:HG22 | 1:M:289:ASP:O    | 2.14                     | 0.48              |
| 1:H:122:VAL:CG1  | 1:H:155:ILE:HD11 | 2.44                     | 0.48              |
| 1:N:210:ARG:HE   | 1:N:244:ARG:HE   | 1.60                     | 0.48              |
| 1:P:115:ARG:CD   | 1:P:134:ASP:OD2  | 2.61                     | 0.48              |
| 1:A:286:LYS:HE3  | 1:B:275:ASP:OD1  | 2.13                     | 0.48              |
| 1:C:205:ASP:OD1  | 1:C:244:ARG:NH1  | 2.47                     | 0.48              |
| 1:D:47:VAL:HG22  | 1:D:94:GLU:HG3   | 1.95                     | 0.48              |
| 1:F:51:THR:HB    | 1:G:88:VAL:HG13  | 1.95                     | 0.48              |
| 1:P:172:HIS:HD2  | 1:P:175:ARG:H    | 1.61                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:60:ILE:HG13  | 1:I:79:TYR:HD1   | 1.77                     | 0.47              |
| 1:N:210:ARG:HH21 | 1:N:244:ARG:HH21 | 1.62                     | 0.47              |
| 1:R:225:TYR:CE1  | 1:R:233:TYR:HB2  | 2.49                     | 0.47              |
| 1:C:168:ILE:HD11 | 1:C:202:LEU:HD13 | 1.97                     | 0.47              |
| 1:H:238:THR:O    | 1:H:244:ARG:NH2  | 2.47                     | 0.47              |
| 1:R:228:ASP:C    | 2:R:301:MBO:HE3  | 2.76                     | 0.47              |
| 1:D:146:PRO:HB3  | 1:D:149:ILE:HD11 | 1.97                     | 0.47              |
| 1:G:246:ALA:HB2  | 1:G:264:LYS:HE3  | 1.96                     | 0.47              |
| 1:L:33:SER:HB3   | 1:L:109:PRO:HD3  | 1.95                     | 0.47              |
| 1:H:53:THR:HG23  | 1:H:88:VAL:HG22  | 1.97                     | 0.47              |
| 1:J:191:THR:HA   | 1:J:281:VAL:HG23 | 1.96                     | 0.47              |
| 1:M:42:LYS:HE3   | 1:M:130:MET:CE   | 2.44                     | 0.47              |
| 1:A:76:GLU:HB3   | 1:I:63:THR:OG1   | 2.14                     | 0.47              |
| 1:C:41:THR:HG23  | 1:C:100:VAL:HG22 | 1.96                     | 0.47              |
| 1:D:20:TRP:HA    | 1:D:118:LEU:HB3  | 1.97                     | 0.47              |
| 1:E:14:VAL:HG12  | 1:E:155:ILE:CD1  | 2.44                     | 0.47              |
| 1:G:238:THR:O    | 1:G:244:ARG:NH2  | 2.48                     | 0.47              |
| 1:L:84:GLN:HG3   | 1:M:55:THR:HG23  | 1.97                     | 0.47              |
| 1:P:103:HIS:NE2  | 1:R:36:GLN:HG3   | 2.30                     | 0.47              |
| 1:D:20:TRP:HB2   | 1:D:147:GLN:HA   | 1.96                     | 0.46              |
| 1:G:24:TYR:CZ    | 1:H:101:ILE:HD11 | 2.50                     | 0.46              |
| 1:N:249:LYS:HE2  | 1:N:257:ASP:OD2  | 2.14                     | 0.46              |
| 1:O:162:ILE:HG23 | 1:O:165:LYS:HB3  | 1.97                     | 0.46              |
| 1:H:240:ASN:HD22 | 1:H:241:PRO:HD2  | 1.80                     | 0.46              |
| 1:D:118:LEU:HD21 | 1:D:133:ILE:HD12 | 1.98                     | 0.46              |
| 1:G:115:ARG:HG3  | 1:G:115:ARG:NH1  | 2.21                     | 0.46              |
| 1:S:31:SER:HA    | 1:S:109:PRO:HB3  | 1.98                     | 0.46              |
| 1:J:203:TYR:HE1  | 1:J:212:LYS:HD3  | 1.79                     | 0.46              |
| 1:S:20:TRP:HB2   | 1:S:147:GLN:HA   | 1.96                     | 0.46              |
| 1:D:40:ILE:HG22  | 1:E:99:LYS:HG3   | 1.97                     | 0.46              |
| 1:F:288:GLU:O    | 1:F:288:GLU:HG3  | 2.16                     | 0.46              |
| 1:L:72:ILE:HG23  | 1:L:73:GLY:H     | 1.81                     | 0.46              |
| 1:A:241:PRO:HB2  | 1:A:265:TYR:HB2  | 1.98                     | 0.46              |
| 1:C:125:ALA:HB2  | 1:C:155:ILE:HD13 | 1.98                     | 0.46              |
| 1:E:109:PRO:O    | 1:E:110:THR:HG22 | 2.16                     | 0.46              |
| 1:F:36:GLN:HG3   | 1:G:103:HIS:CE1  | 2.50                     | 0.46              |
| 1:H:65:SER:O     | 1:I:74:SER:N     | 2.48                     | 0.46              |
| 1:K:269:SER:CB   | 2:K:301:MBO:HE2  | 2.84                     | 0.46              |
| 1:N:33:SER:HB3   | 1:N:109:PRO:HD3  | 1.96                     | 0.46              |
| 1:E:27:GLU:OE1   | 1:E:29:ARG:NH1   | 2.45                     | 0.46              |
| 1:M:87:GLN:OE1   | 1:N:52:ARG:HB3   | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:103:HIS:NE2  | 1:I:36:GLN:HG3   | 2.31                     | 0.46              |
| 1:B:45:LYS:HG3   | 1:B:96:TYR:HB3   | 1.97                     | 0.46              |
| 1:C:118:LEU:HD11 | 1:C:133:ILE:HD12 | 1.98                     | 0.46              |
| 1:D:191:THR:HA   | 1:D:281:VAL:HG23 | 1.98                     | 0.46              |
| 1:E:269:SER:CB   | 2:E:301:MBO:HE6  | 2.84                     | 0.46              |
| 1:P:276:GLY:O    | 1:R:286:LYS:HE3  | 2.16                     | 0.46              |
| 1:S:260:THR:HG22 | 1:S:290:LYS:HA   | 1.98                     | 0.46              |
| 1:J:73:GLY:HA3   | 1:K:66:THR:HA    | 1.97                     | 0.46              |
| 1:A:189:ALA:HA   | 1:A:233:TYR:HA   | 1.98                     | 0.45              |
| 1:C:20:TRP:HB2   | 1:C:147:GLN:HA   | 1.98                     | 0.45              |
| 1:E:266:PHE:HB3  | 2:E:301:MBO:HE6  | 2.36                     | 0.45              |
| 1:H:45:LYS:HG3   | 1:H:96:TYR:HB3   | 1.98                     | 0.45              |
| 1:C:65:SER:HB2   | 1:C:76:GLU:HG2   | 1.99                     | 0.45              |
| 1:E:269:SER:OG   | 2:E:301:MBO:HE6  | 2.55                     | 0.45              |
| 1:M:46:ASN:O     | 1:M:94:GLU:HA    | 2.16                     | 0.45              |
| 1:R:47:VAL:HG22  | 1:R:94:GLU:HG3   | 1.98                     | 0.45              |
| 1:A:210:ARG:HD3  | 1:A:244:ARG:HE   | 1.81                     | 0.45              |
| 1:G:14:VAL:HG22  | 1:G:155:ILE:CD1  | 2.46                     | 0.45              |
| 1:G:159:ARG:HH11 | 1:G:159:ARG:HB2  | 1.80                     | 0.45              |
| 1:G:162:ILE:HG23 | 1:G:165:LYS:HB3  | 1.97                     | 0.45              |
| 1:K:51:THR:HG23  | 1:K:90:MET:HB3   | 1.98                     | 0.45              |
| 1:K:192:LEU:HD22 | 1:K:273:TYR:HD1  | 1.81                     | 0.45              |
| 1:G:41:THR:HG23  | 1:G:100:VAL:HG22 | 1.97                     | 0.45              |
| 1:G:228:ASP:O    | 2:G:301:MBO:HE3  | 2.54                     | 0.45              |
| 1:L:108:PRO:O    | 1:L:111:SER:HB2  | 2.16                     | 0.45              |
| 1:O:53:THR:HG23  | 1:O:88:VAL:HG22  | 1.97                     | 0.45              |
| 1:B:195:SER:OG   | 1:B:197:LEU:HB2  | 2.16                     | 0.45              |
| 1:P:68:ASP:C     | 1:P:70:PHE:H     | 2.25                     | 0.45              |
| 1:D:117:GLN:HE21 | 1:D:130:MET:HG3  | 1.82                     | 0.45              |
| 1:H:227:SER:C    | 1:H:229:GLN:H    | 2.25                     | 0.45              |
| 1:J:68:ASP:C     | 1:J:70:PHE:H     | 2.25                     | 0.45              |
| 1:D:25:VAL:HG22  | 1:D:114:THR:HG22 | 1.99                     | 0.45              |
| 1:D:39:THR:HB    | 1:D:102:GLU:HG3  | 1.98                     | 0.45              |
| 1:G:31:SER:O     | 1:M:109:PRO:HD2  | 2.16                     | 0.45              |
| 1:K:209:PHE:HZ   | 1:K:251:LEU:HD11 | 1.82                     | 0.45              |
| 1:M:18:ALA:HB1   | 1:M:118:LEU:HB3  | 1.99                     | 0.45              |
| 1:N:13:GLU:CG    | 1:N:154:LYS:HE2  | 2.39                     | 0.45              |
| 1:S:273:TYR:HD1  | 1:S:280:ASN:HD22 | 1.62                     | 0.45              |
| 1:E:53:THR:HG23  | 1:E:88:VAL:HG22  | 1.97                     | 0.45              |
| 1:F:37:LYS:HB3   | 1:G:102:GLU:HG2  | 1.98                     | 0.45              |
| 1:F:51:THR:HB    | 1:G:88:VAL:CG1   | 2.47                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:122:VAL:HG11 | 1:L:155:ILE:CD1  | 2.37                     | 0.45              |
| 1:M:53:THR:HG23  | 1:M:88:VAL:HG22  | 1.98                     | 0.45              |
| 1:O:45:LYS:HG3   | 1:O:96:TYR:HB3   | 1.98                     | 0.45              |
| 1:P:53:THR:HG23  | 1:P:88:VAL:HG22  | 1.97                     | 0.45              |
| 1:B:225:TYR:CD1  | 1:B:235:ASP:HB2  | 2.52                     | 0.45              |
| 1:G:115:ARG:HH11 | 1:G:115:ARG:CG   | 2.24                     | 0.45              |
| 1:M:217:MET:HG2  | 1:M:218:TYR:CE2  | 2.52                     | 0.45              |
| 1:N:113:PHE:CD2  | 1:N:113:PHE:C    | 2.94                     | 0.45              |
| 1:O:99:LYS:HE3   | 1:O:101:ILE:HD11 | 1.98                     | 0.45              |
| 1:O:278:ALA:HB1  | 1:P:268:ARG:HD2  | 1.99                     | 0.44              |
| 1:E:36:GLN:NE2   | 1:F:103:HIS:NE2  | 2.61                     | 0.44              |
| 1:J:277:PRO:HD2  | 1:J:282:TYR:OH   | 2.17                     | 0.44              |
| 1:A:232:ILE:HD11 | 1:A:283:CYS:HB2  | 1.98                     | 0.44              |
| 1:C:232:ILE:HD11 | 1:C:283:CYS:HB2  | 1.99                     | 0.44              |
| 1:O:203:TYR:HE1  | 1:O:212:LYS:HD3  | 1.83                     | 0.44              |
| 1:L:34:VAL:HG23  | 1:L:107:ILE:HB   | 1.98                     | 0.44              |
| 1:L:85:LYS:HG2   | 1:M:54:VAL:HG22  | 1.99                     | 0.44              |
| 1:E:183:SER:HB2  | 1:E:217:MET:HE3  | 1.99                     | 0.44              |
| 1:E:232:ILE:HD11 | 1:E:283:CYS:HB2  | 1.99                     | 0.44              |
| 1:K:105:ILE:HB   | 1:L:34:VAL:HG12  | 1.99                     | 0.44              |
| 1:N:31:SER:HA    | 1:N:109:PRO:HB3  | 1.98                     | 0.44              |
| 1:D:225:TYR:CD1  | 1:D:235:ASP:HB2  | 2.53                     | 0.44              |
| 1:D:269:SER:CB   | 2:D:301:MBO:HE6  | 2.86                     | 0.44              |
| 1:G:192:LEU:HD22 | 1:G:273:TYR:HD1  | 1.83                     | 0.44              |
| 1:H:188:PRO:HD3  | 1:H:218:TYR:HD1  | 1.82                     | 0.44              |
| 1:K:268:ARG:HH11 | 1:K:268:ARG:HB2  | 1.82                     | 0.44              |
| 1:A:67:GLY:C     | 1:A:69:ALA:N     | 2.76                     | 0.44              |
| 1:D:255:HIS:CE1  | 1:D:294:GLU:HB3  | 2.53                     | 0.44              |
| 1:G:268:ARG:HD2  | 1:H:278:ALA:HB1  | 2.00                     | 0.44              |
| 1:K:249:LYS:HE2  | 1:K:257:ASP:OD2  | 2.18                     | 0.44              |
| 1:L:84:GLN:HE21  | 1:L:84:GLN:HB2   | 1.61                     | 0.44              |
| 1:L:238:THR:O    | 1:L:244:ARG:NH2  | 2.51                     | 0.44              |
| 1:N:85:LYS:HG2   | 1:O:54:VAL:HG22  | 1.98                     | 0.44              |
| 1:P:17:VAL:HG13  | 1:P:150:THR:HG22 | 1.99                     | 0.44              |
| 1:A:52:ARG:HG2   | 1:B:87:GLN:OE1   | 2.17                     | 0.44              |
| 1:C:171:LYS:HD3  | 1:C:176:LYS:HG2  | 2.00                     | 0.44              |
| 1:F:20:TRP:HB2   | 1:F:147:GLN:HA   | 1.99                     | 0.44              |
| 1:S:266:PHE:HB2  | 1:S:269:SER:OG   | 2.18                     | 0.44              |
| 1:B:269:SER:CB   | 2:B:302:MBO:HE6  | 2.87                     | 0.43              |
| 1:O:115:ARG:HD3  | 1:O:134:ASP:OD2  | 2.17                     | 0.43              |
| 1:O:278:ALA:HB1  | 1:P:268:ARG:CD   | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:199:LYS:HD3  | 1:E:296:VAL:HG11 | 1.99                     | 0.43              |
| 1:F:50:GLU:O     | 1:F:90:MET:HA    | 2.18                     | 0.43              |
| 1:I:162:ILE:HG13 | 1:I:165:LYS:HB3  | 2.00                     | 0.43              |
| 1:J:18:ALA:HA    | 1:J:120:ALA:HA   | 2.00                     | 0.43              |
| 1:N:99:LYS:HG3   | 1:O:40:ILE:HG22  | 1.99                     | 0.43              |
| 1:R:103:HIS:NE2  | 1:S:36:GLN:HG3   | 2.33                     | 0.43              |
| 1:D:34:VAL:HG12  | 1:E:105:ILE:HB   | 1.99                     | 0.43              |
| 1:E:41:THR:HG23  | 1:E:100:VAL:HG22 | 2.01                     | 0.43              |
| 1:L:188:PRO:HG2  | 1:L:234:PHE:HB2  | 2.00                     | 0.43              |
| 1:G:115:ARG:HG3  | 1:G:134:ASP:OD2  | 2.18                     | 0.43              |
| 1:H:122:VAL:HG11 | 1:H:155:ILE:HD11 | 2.01                     | 0.43              |
| 1:G:203:TYR:HB2  | 1:G:210:ARG:HB2  | 1.99                     | 0.43              |
| 1:H:62:SER:HB2   | 1:I:77:VAL:HG22  | 2.00                     | 0.43              |
| 1:I:175:ARG:NH1  | 1:I:177:GLU:OE1  | 2.51                     | 0.43              |
| 1:M:33:SER:HB3   | 1:M:109:PRO:HD3  | 2.00                     | 0.43              |
| 1:M:240:ASN:HD21 | 1:M:242:LYS:HB2  | 1.83                     | 0.43              |
| 1:M:268:ARG:NH1  | 1:M:285:ASP:OD2  | 2.52                     | 0.43              |
| 1:N:249:LYS:HB3  | 1:N:249:LYS:HE3  | 1.71                     | 0.43              |
| 1:S:225:TYR:HB3  | 1:S:243:GLN:HB3  | 1.99                     | 0.43              |
| 1:P:115:ARG:HD3  | 1:P:134:ASP:OD2  | 2.19                     | 0.43              |
| 1:B:228:ASP:O    | 2:B:302:MBO:HE3  | 2.57                     | 0.43              |
| 1:F:191:THR:HA   | 1:F:281:VAL:HG23 | 2.00                     | 0.43              |
| 1:F:236:GLN:O    | 1:F:238:THR:HG23 | 2.19                     | 0.43              |
| 2:G:301:MBO:HE5  | 2:G:301:MBO:OZ2  | 2.51                     | 0.43              |
| 1:L:103:HIS:NE2  | 1:M:36:GLN:HG3   | 2.33                     | 0.43              |
| 1:G:18:ALA:HA    | 1:G:120:ALA:HA   | 2.01                     | 0.43              |
| 1:I:232:ILE:HD11 | 1:I:283:CYS:HB2  | 2.01                     | 0.43              |
| 1:C:16:VAL:HG12  | 1:C:122:VAL:HA   | 2.01                     | 0.43              |
| 1:M:67:GLY:C     | 1:M:69:ALA:H     | 2.27                     | 0.43              |
| 1:C:223:TYR:O    | 1:C:234:PHE:HA   | 2.19                     | 0.42              |
| 2:G:301:MBO:HE3  | 2:G:301:MBO:OZ1  | 2.57                     | 0.42              |
| 2:P:302:MBO:HE3  | 2:P:302:MBO:OZ2  | 2.56                     | 0.42              |
| 1:B:142:THR:HG21 | 1:C:152:ARG:HB2  | 2.01                     | 0.42              |
| 1:C:269:SER:HB3  | 2:C:301:MBO:HE6  | 2.38                     | 0.42              |
| 1:E:113:PHE:CD2  | 1:E:113:PHE:C    | 2.97                     | 0.42              |
| 1:F:55:THR:HG23  | 1:G:84:GLN:HB3   | 2.00                     | 0.42              |
| 1:E:25:VAL:HG22  | 1:E:114:THR:HG22 | 2.00                     | 0.42              |
| 1:I:31:SER:HA    | 1:I:109:PRO:HB3  | 2.01                     | 0.42              |
| 1:A:158:GLY:N    | 1:I:148:VAL:HG13 | 2.35                     | 0.42              |
| 1:D:162:ILE:HG23 | 1:D:165:LYS:HB3  | 2.02                     | 0.42              |
| 1:D:188:PRO:HD3  | 1:D:218:TYR:HD1  | 1.84                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:18:ALA:HA    | 1:H:120:ALA:HA   | 2.01                     | 0.42              |
| 1:H:205:ASP:OD2  | 1:H:244:ARG:NH1  | 2.51                     | 0.42              |
| 1:J:55:THR:HG23  | 1:S:84:GLN:HB3   | 2.01                     | 0.42              |
| 1:K:107:ILE:HA   | 1:K:108:PRO:HD3  | 1.90                     | 0.42              |
| 1:L:245:TRP:CH2  | 1:L:271:LEU:HD13 | 2.55                     | 0.42              |
| 2:L:301:MBO:HE3  | 2:L:301:MBO:OZ1  | 2.57                     | 0.42              |
| 1:N:48:ASN:HB2   | 1:N:93:THR:CG2   | 2.48                     | 0.42              |
| 1:P:115:ARG:HD2  | 1:P:134:ASP:OD2  | 2.19                     | 0.42              |
| 1:P:162:ILE:HD12 | 1:P:166:THR:HG23 | 2.01                     | 0.42              |
| 1:C:251:LEU:HB3  | 1:C:252:PRO:HA   | 2.02                     | 0.42              |
| 1:D:146:PRO:HB2  | 1:D:149:ILE:CD1  | 2.49                     | 0.42              |
| 1:H:188:PRO:HG2  | 1:H:234:PHE:HB2  | 2.01                     | 0.42              |
| 1:H:269:SER:HB2  | 1:H:284:LEU:C    | 2.45                     | 0.42              |
| 1:J:232:ILE:HD11 | 1:J:283:CYS:HB2  | 2.00                     | 0.42              |
| 1:L:205:ASP:OD2  | 1:L:244:ARG:NH1  | 2.53                     | 0.42              |
| 1:O:225:TYR:CD1  | 1:O:235:ASP:HB2  | 2.54                     | 0.42              |
| 1:P:188:PRO:HG2  | 1:P:234:PHE:HB2  | 2.01                     | 0.42              |
| 1:R:175:ARG:NH1  | 1:R:177:GLU:OE1  | 2.53                     | 0.42              |
| 1:R:225:TYR:CD1  | 1:R:235:ASP:HB2  | 2.55                     | 0.42              |
| 1:E:152:ARG:HD3  | 1:E:152:ARG:HA   | 1.82                     | 0.42              |
| 1:O:285:ASP:OD1  | 2:O:301:MBO:HE5  | 2.58                     | 0.42              |
| 1:A:63:THR:HG23  | 1:A:78:SER:HB3   | 2.02                     | 0.42              |
| 1:K:152:ARG:HB2  | 1:L:142:THR:HG21 | 2.02                     | 0.42              |
| 1:K:260:THR:HG22 | 1:K:290:LYS:HA   | 2.01                     | 0.42              |
| 1:M:157:VAL:HB   | 1:M:254:ARG:HD3  | 2.01                     | 0.42              |
| 1:B:243:GLN:HE21 | 1:B:244:ARG:HE   | 1.68                     | 0.42              |
| 1:C:65:SER:CB    | 1:C:76:GLU:HG2   | 2.50                     | 0.42              |
| 1:N:248:ASN:HB3  | 1:N:260:THR:CG2  | 2.50                     | 0.41              |
| 1:P:260:THR:HG22 | 1:P:290:LYS:HA   | 2.02                     | 0.41              |
| 1:B:272:CYS:HA   | 1:B:289:ASP:HB2  | 2.02                     | 0.41              |
| 1:E:45:LYS:HB3   | 1:F:94:GLU:HB2   | 2.02                     | 0.41              |
| 1:J:113:PHE:CD2  | 1:J:113:PHE:C    | 2.98                     | 0.41              |
| 1:A:92:GLN:HE21  | 1:A:92:GLN:HB2   | 1.62                     | 0.41              |
| 1:F:14:VAL:CG1   | 1:F:155:ILE:HD13 | 2.47                     | 0.41              |
| 1:S:210:ARG:HG2  | 1:S:223:TYR:HD2  | 1.85                     | 0.41              |
| 1:D:269:SER:OG   | 2:D:301:MBO:HE6  | 2.58                     | 0.41              |
| 1:L:115:ARG:HD3  | 1:L:134:ASP:OD2  | 2.20                     | 0.41              |
| 1:M:96:TYR:CZ    | 1:N:43:GLY:HA3   | 2.55                     | 0.41              |
| 2:P:302:MBO:HE5  | 2:P:302:MBO:OZ1  | 2.57                     | 0.41              |
| 1:F:24:TYR:OH    | 1:F:36:GLN:NE2   | 2.53                     | 0.41              |
| 1:A:18:ALA:HA    | 1:A:120:ALA:HA   | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:183:SER:HB2  | 1:J:217:MET:HE3  | 2.02                     | 0.41              |
| 2:K:302:MBO:HE5  | 2:K:302:MBO:OZ2  | 2.58                     | 0.41              |
| 1:L:248:ASN:HB3  | 1:L:260:THR:CG2  | 2.50                     | 0.41              |
| 1:M:152:ARG:HA   | 1:M:152:ARG:HD2  | 1.88                     | 0.41              |
| 1:O:22:GLU:HB3   | 1:O:117:GLN:HG2  | 2.01                     | 0.41              |
| 1:A:110:THR:O    | 1:A:110:THR:HG23 | 2.20                     | 0.41              |
| 1:J:207:GLY:HA3  | 1:J:244:ARG:HD3  | 2.01                     | 0.41              |
| 1:J:188:PRO:HG2  | 1:J:234:PHE:HB2  | 2.03                     | 0.41              |
| 1:R:260:THR:HG22 | 1:R:290:LYS:HA   | 2.01                     | 0.41              |
| 1:B:243:GLN:HE22 | 1:B:244:ARG:HH21 | 1.67                     | 0.41              |
| 1:D:146:PRO:HB2  | 1:D:149:ILE:HD11 | 2.01                     | 0.41              |
| 1:G:266:PHE:HB3  | 2:G:301:MBO:HE6  | 2.41                     | 0.41              |
| 1:I:269:SER:HB3  | 2:I:302:MBO:HE2  | 2.41                     | 0.41              |
| 1:J:157:VAL:HB   | 1:J:254:ARG:HD3  | 2.03                     | 0.41              |
| 1:P:152:ARG:HB2  | 1:R:142:THR:HG21 | 2.02                     | 0.41              |
| 1:R:223:TYR:O    | 1:R:234:PHE:HA   | 2.21                     | 0.41              |
| 1:C:203:TYR:HE1  | 1:C:212:LYS:HD3  | 1.86                     | 0.41              |
| 1:D:64:ILE:HG12  | 1:E:75:VAL:HG23  | 2.03                     | 0.41              |
| 1:E:201:VAL:HG12 | 1:E:214:LEU:HD21 | 2.03                     | 0.41              |
| 1:E:241:PRO:HB2  | 1:E:265:TYR:HB2  | 2.03                     | 0.41              |
| 1:J:241:PRO:HB2  | 1:J:265:TYR:HB2  | 2.02                     | 0.41              |
| 1:K:45:LYS:HE2   | 1:K:45:LYS:HB3   | 1.91                     | 0.41              |
| 2:L:301:MBO:HE5  | 2:L:301:MBO:OZ2  | 2.59                     | 0.41              |
| 1:P:266:PHE:CB   | 2:P:302:MBO:HE6  | 2.89                     | 0.41              |
| 1:R:80:SER:OG    | 1:S:59:SER:HB2   | 2.21                     | 0.41              |
| 1:S:106:THR:O    | 1:S:108:PRO:HD3  | 2.21                     | 0.41              |
| 1:A:117:GLN:HG3  | 1:A:132:LEU:CD2  | 2.51                     | 0.40              |
| 1:D:47:VAL:HA    | 1:D:93:THR:O     | 2.22                     | 0.40              |
| 1:O:90:MET:HB2   | 1:P:49:SER:HB2   | 2.02                     | 0.40              |
| 1:O:164:GLY:HA2  | 1:O:203:TYR:CE2  | 2.56                     | 0.40              |
| 1:A:53:THR:HG23  | 1:A:88:VAL:HG12  | 2.03                     | 0.40              |
| 1:B:164:GLY:HA2  | 1:B:203:TYR:CE2  | 2.56                     | 0.40              |
| 1:D:241:PRO:HB2  | 1:D:265:TYR:HB2  | 2.02                     | 0.40              |
| 1:F:49:SER:HB3   | 1:G:90:MET:HB3   | 2.03                     | 0.40              |
| 1:F:232:ILE:HD11 | 1:F:283:CYS:HB2  | 2.02                     | 0.40              |
| 1:H:240:ASN:HA   | 1:H:241:PRO:HD2  | 1.88                     | 0.40              |
| 1:K:269:SER:HG   | 2:K:301:MBO:HE2  | 2.25                     | 0.40              |
| 1:N:277:PRO:HD2  | 1:N:282:TYR:OH   | 2.20                     | 0.40              |
| 1:R:92:GLN:HB3   | 1:S:47:VAL:HB    | 2.04                     | 0.40              |
| 1:R:112:LYS:HE2  | 1:R:112:LYS:HB3  | 1.95                     | 0.40              |
| 1:I:37:LYS:HA    | 1:I:103:HIS:O    | 2.21                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:J:212:LYS:HA  | 1:J:222:GLU:O   | 2.21                     | 0.40              |
| 1:M:172:HIS:CD2 | 1:M:175:ARG:HB2 | 2.56                     | 0.40              |
| 1:R:266:PHE:HB3 | 1:R:269:SER:OG  | 2.20                     | 0.40              |
| 1:A:286:LYS:HE2 | 1:A:286:LYS:HB2 | 1.87                     | 0.40              |
| 1:K:36:GLN:HG2  | 1:K:107:ILE:CD1 | 2.52                     | 0.40              |
| 1:O:157:VAL:HB  | 1:O:254:ARG:HD3 | 2.03                     | 0.40              |
| 1:F:268:ARG:HD2 | 1:G:278:ALA:HB1 | 2.04                     | 0.40              |
| 1:I:51:THR:HG23 | 1:I:90:MET:HB3  | 2.03                     | 0.40              |
| 1:M:67:GLY:O    | 1:M:69:ALA:N    | 2.54                     | 0.40              |
| 1:R:33:SER:HB3  | 1:R:109:PRO:HD3 | 2.04                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:F:239:ASP:OD2 | 1:R:236:GLN:OE1[7_556] | 1.52                     | 0.68              |

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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   | A     | 288/298 (97%) | 273 (95%) | 12 (4%) | 3 (1%)   | 12          | 41  |
| 1   | B     | 280/298 (94%) | 269 (96%) | 11 (4%) | 0        | 100         | 100 |
| 1   | C     | 282/298 (95%) | 269 (95%) | 13 (5%) | 0        | 100         | 100 |
| 1   | D     | 281/298 (94%) | 272 (97%) | 8 (3%)  | 1 (0%)   | 30          | 61  |
| 1   | E     | 279/298 (94%) | 267 (96%) | 12 (4%) | 0        | 100         | 100 |
| 1   | F     | 279/298 (94%) | 259 (93%) | 18 (6%) | 2 (1%)   | 18          | 49  |
| 1   | G     | 288/298 (97%) | 273 (95%) | 11 (4%) | 4 (1%)   | 9           | 34  |
| 1   | H     | 279/298 (94%) | 272 (98%) | 7 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | I     | 278/298 (93%)   | 269 (97%)  | 9 (3%)   | 0        | 100         | 100 |
| 1   | J     | 288/298 (97%)   | 274 (95%)  | 11 (4%)  | 3 (1%)   | 12          | 41  |
| 1   | K     | 288/298 (97%)   | 272 (94%)  | 13 (4%)  | 3 (1%)   | 12          | 41  |
| 1   | L     | 280/298 (94%)   | 268 (96%)  | 12 (4%)  | 0        | 100         | 100 |
| 1   | M     | 287/298 (96%)   | 265 (92%)  | 20 (7%)  | 2 (1%)   | 18          | 49  |
| 1   | N     | 287/298 (96%)   | 270 (94%)  | 16 (6%)  | 1 (0%)   | 36          | 67  |
| 1   | O     | 287/298 (96%)   | 274 (96%)  | 10 (4%)  | 3 (1%)   | 12          | 41  |
| 1   | P     | 287/298 (96%)   | 270 (94%)  | 15 (5%)  | 2 (1%)   | 18          | 49  |
| 1   | R     | 279/298 (94%)   | 270 (97%)  | 9 (3%)   | 0        | 100         | 100 |
| 1   | S     | 279/298 (94%)   | 263 (94%)  | 15 (5%)  | 1 (0%)   | 30          | 61  |
| All | All   | 5096/5364 (95%) | 4849 (95%) | 222 (4%) | 25 (0%)  | 24          | 57  |

All (25) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 68  | ASP  |
| 1   | A     | 70  | PHE  |
| 1   | A     | 71  | GLU  |
| 1   | G     | 68  | ASP  |
| 1   | G     | 72  | ILE  |
| 1   | K     | 68  | ASP  |
| 1   | K     | 71  | GLU  |
| 1   | O     | 68  | ASP  |
| 1   | O     | 71  | GLU  |
| 1   | P     | 72  | ILE  |
| 1   | S     | 143 | GLN  |
| 1   | K     | 72  | ILE  |
| 1   | N     | 72  | ILE  |
| 1   | O     | 72  | ILE  |
| 1   | P     | 69  | ALA  |
| 1   | G     | 71  | GLU  |
| 1   | M     | 68  | ASP  |
| 1   | F     | 110 | THR  |
| 1   | J     | 71  | GLU  |
| 1   | M     | 70  | PHE  |
| 1   | F     | 237 | GLY  |
| 1   | G     | 228 | ASP  |
| 1   | J     | 68  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 69  | ALA  |
| 1   | D     | 146 | PRO  |

### 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   | A     | 253/257 (98%)   | 220 (87%)  | 33 (13%)  | 4           | 18 |
| 1   | B     | 250/257 (97%)   | 226 (90%)  | 24 (10%)  | 8           | 30 |
| 1   | C     | 250/257 (97%)   | 223 (89%)  | 27 (11%)  | 6           | 25 |
| 1   | D     | 250/257 (97%)   | 220 (88%)  | 30 (12%)  | 5           | 21 |
| 1   | E     | 249/257 (97%)   | 218 (88%)  | 31 (12%)  | 4           | 19 |
| 1   | F     | 249/257 (97%)   | 217 (87%)  | 32 (13%)  | 4           | 18 |
| 1   | G     | 253/257 (98%)   | 223 (88%)  | 30 (12%)  | 5           | 21 |
| 1   | H     | 249/257 (97%)   | 221 (89%)  | 28 (11%)  | 6           | 24 |
| 1   | I     | 249/257 (97%)   | 218 (88%)  | 31 (12%)  | 4           | 19 |
| 1   | J     | 253/257 (98%)   | 222 (88%)  | 31 (12%)  | 4           | 20 |
| 1   | K     | 253/257 (98%)   | 219 (87%)  | 34 (13%)  | 4           | 17 |
| 1   | L     | 250/257 (97%)   | 227 (91%)  | 23 (9%)   | 8           | 31 |
| 1   | M     | 253/257 (98%)   | 229 (90%)  | 24 (10%)  | 8           | 30 |
| 1   | N     | 253/257 (98%)   | 224 (88%)  | 29 (12%)  | 5           | 23 |
| 1   | O     | 253/257 (98%)   | 228 (90%)  | 25 (10%)  | 7           | 29 |
| 1   | P     | 253/257 (98%)   | 220 (87%)  | 33 (13%)  | 4           | 18 |
| 1   | R     | 249/257 (97%)   | 224 (90%)  | 25 (10%)  | 7           | 29 |
| 1   | S     | 249/257 (97%)   | 224 (90%)  | 25 (10%)  | 7           | 29 |
| All | All   | 4518/4626 (98%) | 4003 (89%) | 515 (11%) | 5           | 23 |

All (515) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 15  | ASP  |
| 1   | A     | 16  | VAL  |
| 1   | A     | 42  | LYS  |
| 1   | A     | 45  | LYS  |
| 1   | A     | 47  | VAL  |
| 1   | A     | 57  | THR  |
| 1   | A     | 62  | SER  |
| 1   | A     | 63  | THR  |
| 1   | A     | 68  | ASP  |
| 1   | A     | 71  | GLU  |
| 1   | A     | 78  | SER  |
| 1   | A     | 88  | VAL  |
| 1   | A     | 98  | SER  |
| 1   | A     | 100 | VAL  |
| 1   | A     | 110 | THR  |
| 1   | A     | 148 | VAL  |
| 1   | A     | 149 | ILE  |
| 1   | A     | 152 | ARG  |
| 1   | A     | 157 | VAL  |
| 1   | A     | 166 | THR  |
| 1   | A     | 168 | ILE  |
| 1   | A     | 184 | ARG  |
| 1   | A     | 186 | SER  |
| 1   | A     | 191 | THR  |
| 1   | A     | 192 | LEU  |
| 1   | A     | 196 | LYS  |
| 1   | A     | 201 | VAL  |
| 1   | A     | 211 | ILE  |
| 1   | A     | 244 | ARG  |
| 1   | A     | 251 | LEU  |
| 1   | A     | 254 | ARG  |
| 1   | A     | 260 | THR  |
| 1   | A     | 287 | ARG  |
| 1   | B     | 15  | ASP  |
| 1   | B     | 16  | VAL  |
| 1   | B     | 39  | THR  |
| 1   | B     | 44  | MET  |
| 1   | B     | 51  | THR  |
| 1   | B     | 53  | THR  |
| 1   | B     | 57  | THR  |
| 1   | B     | 62  | SER  |
| 1   | B     | 84  | GLN  |
| 1   | B     | 90  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 93  | THR  |
| 1   | B     | 110 | THR  |
| 1   | B     | 118 | LEU  |
| 1   | B     | 143 | GLN  |
| 1   | B     | 148 | VAL  |
| 1   | B     | 174 | GLU  |
| 1   | B     | 191 | THR  |
| 1   | B     | 192 | LEU  |
| 1   | B     | 197 | LEU  |
| 1   | B     | 211 | ILE  |
| 1   | B     | 243 | GLN  |
| 1   | B     | 244 | ARG  |
| 1   | B     | 260 | THR  |
| 1   | B     | 290 | LYS  |
| 1   | C     | 13  | GLU  |
| 1   | C     | 15  | ASP  |
| 1   | C     | 32  | THR  |
| 1   | C     | 36  | GLN  |
| 1   | C     | 39  | THR  |
| 1   | C     | 44  | MET  |
| 1   | C     | 53  | THR  |
| 1   | C     | 55  | THR  |
| 1   | C     | 57  | THR  |
| 1   | C     | 60  | ILE  |
| 1   | C     | 63  | THR  |
| 1   | C     | 66  | THR  |
| 1   | C     | 68  | ASP  |
| 1   | C     | 84  | GLN  |
| 1   | C     | 88  | VAL  |
| 1   | C     | 92  | GLN  |
| 1   | C     | 98  | SER  |
| 1   | C     | 104 | THR  |
| 1   | C     | 110 | THR  |
| 1   | C     | 115 | ARG  |
| 1   | C     | 150 | THR  |
| 1   | C     | 176 | LYS  |
| 1   | C     | 191 | THR  |
| 1   | C     | 192 | LEU  |
| 1   | C     | 219 | SER  |
| 1   | C     | 229 | GLN  |
| 1   | C     | 244 | ARG  |
| 1   | D     | 15  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 16  | VAL  |
| 1   | D     | 17  | VAL  |
| 1   | D     | 39  | THR  |
| 1   | D     | 52  | ARG  |
| 1   | D     | 53  | THR  |
| 1   | D     | 55  | THR  |
| 1   | D     | 57  | THR  |
| 1   | D     | 59  | SER  |
| 1   | D     | 88  | VAL  |
| 1   | D     | 90  | MET  |
| 1   | D     | 93  | THR  |
| 1   | D     | 98  | SER  |
| 1   | D     | 118 | LEU  |
| 1   | D     | 145 | ILE  |
| 1   | D     | 148 | VAL  |
| 1   | D     | 159 | ARG  |
| 1   | D     | 165 | LYS  |
| 1   | D     | 174 | GLU  |
| 1   | D     | 191 | THR  |
| 1   | D     | 192 | LEU  |
| 1   | D     | 197 | LEU  |
| 1   | D     | 201 | VAL  |
| 1   | D     | 211 | ILE  |
| 1   | D     | 229 | GLN  |
| 1   | D     | 260 | THR  |
| 1   | D     | 271 | LEU  |
| 1   | D     | 283 | CYS  |
| 1   | D     | 286 | LYS  |
| 1   | D     | 294 | GLU  |
| 1   | E     | 12  | ILE  |
| 1   | E     | 14  | VAL  |
| 1   | E     | 15  | ASP  |
| 1   | E     | 16  | VAL  |
| 1   | E     | 19  | VAL  |
| 1   | E     | 29  | ARG  |
| 1   | E     | 37  | LYS  |
| 1   | E     | 40  | ILE  |
| 1   | E     | 47  | VAL  |
| 1   | E     | 55  | THR  |
| 1   | E     | 57  | THR  |
| 1   | E     | 64  | ILE  |
| 1   | E     | 78  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 90  | MET  |
| 1   | E     | 92  | GLN  |
| 1   | E     | 98  | SER  |
| 1   | E     | 118 | LEU  |
| 1   | E     | 148 | VAL  |
| 1   | E     | 152 | ARG  |
| 1   | E     | 162 | ILE  |
| 1   | E     | 165 | LYS  |
| 1   | E     | 166 | THR  |
| 1   | E     | 184 | ARG  |
| 1   | E     | 186 | SER  |
| 1   | E     | 191 | THR  |
| 1   | E     | 192 | LEU  |
| 1   | E     | 217 | MET  |
| 1   | E     | 229 | GLN  |
| 1   | E     | 244 | ARG  |
| 1   | E     | 260 | THR  |
| 1   | E     | 294 | GLU  |
| 1   | F     | 10  | GLU  |
| 1   | F     | 13  | GLU  |
| 1   | F     | 16  | VAL  |
| 1   | F     | 19  | VAL  |
| 1   | F     | 42  | LYS  |
| 1   | F     | 49  | SER  |
| 1   | F     | 62  | SER  |
| 1   | F     | 66  | THR  |
| 1   | F     | 78  | SER  |
| 1   | F     | 80  | SER  |
| 1   | F     | 88  | VAL  |
| 1   | F     | 90  | MET  |
| 1   | F     | 98  | SER  |
| 1   | F     | 100 | VAL  |
| 1   | F     | 142 | THR  |
| 1   | F     | 148 | VAL  |
| 1   | F     | 154 | LYS  |
| 1   | F     | 159 | ARG  |
| 1   | F     | 166 | THR  |
| 1   | F     | 171 | LYS  |
| 1   | F     | 191 | THR  |
| 1   | F     | 197 | LEU  |
| 1   | F     | 201 | VAL  |
| 1   | F     | 227 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 244 | ARG  |
| 1   | F     | 249 | LYS  |
| 1   | F     | 250 | SER  |
| 1   | F     | 260 | THR  |
| 1   | F     | 264 | LYS  |
| 1   | F     | 267 | THR  |
| 1   | F     | 284 | LEU  |
| 1   | F     | 286 | LYS  |
| 1   | G     | 15  | ASP  |
| 1   | G     | 16  | VAL  |
| 1   | G     | 51  | THR  |
| 1   | G     | 55  | THR  |
| 1   | G     | 57  | THR  |
| 1   | G     | 70  | PHE  |
| 1   | G     | 92  | GLN  |
| 1   | G     | 93  | THR  |
| 1   | G     | 98  | SER  |
| 1   | G     | 106 | THR  |
| 1   | G     | 114 | THR  |
| 1   | G     | 115 | ARG  |
| 1   | G     | 118 | LEU  |
| 1   | G     | 148 | VAL  |
| 1   | G     | 159 | ARG  |
| 1   | G     | 165 | LYS  |
| 1   | G     | 174 | GLU  |
| 1   | G     | 175 | ARG  |
| 1   | G     | 192 | LEU  |
| 1   | G     | 201 | VAL  |
| 1   | G     | 210 | ARG  |
| 1   | G     | 219 | SER  |
| 1   | G     | 229 | GLN  |
| 1   | G     | 244 | ARG  |
| 1   | G     | 247 | ILE  |
| 1   | G     | 260 | THR  |
| 1   | G     | 264 | LYS  |
| 1   | G     | 271 | LEU  |
| 1   | G     | 283 | CYS  |
| 1   | G     | 284 | LEU  |
| 1   | H     | 15  | ASP  |
| 1   | H     | 20  | TRP  |
| 1   | H     | 53  | THR  |
| 1   | H     | 55  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 57  | THR  |
| 1   | H     | 59  | SER  |
| 1   | H     | 62  | SER  |
| 1   | H     | 87  | GLN  |
| 1   | H     | 88  | VAL  |
| 1   | H     | 90  | MET  |
| 1   | H     | 93  | THR  |
| 1   | H     | 98  | SER  |
| 1   | H     | 114 | THR  |
| 1   | H     | 152 | ARG  |
| 1   | H     | 168 | ILE  |
| 1   | H     | 174 | GLU  |
| 1   | H     | 185 | LYS  |
| 1   | H     | 191 | THR  |
| 1   | H     | 192 | LEU  |
| 1   | H     | 197 | LEU  |
| 1   | H     | 201 | VAL  |
| 1   | H     | 229 | GLN  |
| 1   | H     | 244 | ARG  |
| 1   | H     | 247 | ILE  |
| 1   | H     | 260 | THR  |
| 1   | H     | 287 | ARG  |
| 1   | H     | 294 | GLU  |
| 1   | H     | 295 | VAL  |
| 1   | I     | 13  | GLU  |
| 1   | I     | 14  | VAL  |
| 1   | I     | 15  | ASP  |
| 1   | I     | 16  | VAL  |
| 1   | I     | 19  | VAL  |
| 1   | I     | 39  | THR  |
| 1   | I     | 44  | MET  |
| 1   | I     | 48  | ASN  |
| 1   | I     | 55  | THR  |
| 1   | I     | 57  | THR  |
| 1   | I     | 60  | ILE  |
| 1   | I     | 75  | VAL  |
| 1   | I     | 82  | SER  |
| 1   | I     | 93  | THR  |
| 1   | I     | 98  | SER  |
| 1   | I     | 110 | THR  |
| 1   | I     | 112 | LYS  |
| 1   | I     | 118 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 132 | LEU  |
| 1   | I     | 148 | VAL  |
| 1   | I     | 149 | ILE  |
| 1   | I     | 155 | ILE  |
| 1   | I     | 191 | THR  |
| 1   | I     | 192 | LEU  |
| 1   | I     | 201 | VAL  |
| 1   | I     | 229 | GLN  |
| 1   | I     | 244 | ARG  |
| 1   | I     | 250 | SER  |
| 1   | I     | 260 | THR  |
| 1   | I     | 264 | LYS  |
| 1   | I     | 271 | LEU  |
| 1   | J     | 15  | ASP  |
| 1   | J     | 16  | VAL  |
| 1   | J     | 44  | MET  |
| 1   | J     | 47  | VAL  |
| 1   | J     | 49  | SER  |
| 1   | J     | 55  | THR  |
| 1   | J     | 57  | THR  |
| 1   | J     | 62  | SER  |
| 1   | J     | 63  | THR  |
| 1   | J     | 64  | ILE  |
| 1   | J     | 68  | ASP  |
| 1   | J     | 72  | ILE  |
| 1   | J     | 75  | VAL  |
| 1   | J     | 90  | MET  |
| 1   | J     | 93  | THR  |
| 1   | J     | 98  | SER  |
| 1   | J     | 100 | VAL  |
| 1   | J     | 110 | THR  |
| 1   | J     | 121 | ASP  |
| 1   | J     | 148 | VAL  |
| 1   | J     | 159 | ARG  |
| 1   | J     | 186 | SER  |
| 1   | J     | 191 | THR  |
| 1   | J     | 192 | LEU  |
| 1   | J     | 197 | LEU  |
| 1   | J     | 202 | LEU  |
| 1   | J     | 217 | MET  |
| 1   | J     | 229 | GLN  |
| 1   | J     | 250 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 271 | LEU  |
| 1   | J     | 296 | VAL  |
| 1   | K     | 16  | VAL  |
| 1   | K     | 33  | SER  |
| 1   | K     | 36  | GLN  |
| 1   | K     | 42  | LYS  |
| 1   | K     | 47  | VAL  |
| 1   | K     | 55  | THR  |
| 1   | K     | 57  | THR  |
| 1   | K     | 59  | SER  |
| 1   | K     | 66  | THR  |
| 1   | K     | 82  | SER  |
| 1   | K     | 90  | MET  |
| 1   | K     | 98  | SER  |
| 1   | K     | 100 | VAL  |
| 1   | K     | 104 | THR  |
| 1   | K     | 105 | ILE  |
| 1   | K     | 106 | THR  |
| 1   | K     | 110 | THR  |
| 1   | K     | 128 | GLU  |
| 1   | K     | 142 | THR  |
| 1   | K     | 148 | VAL  |
| 1   | K     | 165 | LYS  |
| 1   | K     | 174 | GLU  |
| 1   | K     | 175 | ARG  |
| 1   | K     | 179 | MET  |
| 1   | K     | 184 | ARG  |
| 1   | K     | 192 | LEU  |
| 1   | K     | 229 | GLN  |
| 1   | K     | 232 | ILE  |
| 1   | K     | 264 | LYS  |
| 1   | K     | 268 | ARG  |
| 1   | K     | 271 | LEU  |
| 1   | K     | 286 | LYS  |
| 1   | K     | 287 | ARG  |
| 1   | K     | 290 | LYS  |
| 1   | L     | 13  | GLU  |
| 1   | L     | 16  | VAL  |
| 1   | L     | 21  | LYS  |
| 1   | L     | 34  | VAL  |
| 1   | L     | 39  | THR  |
| 1   | L     | 45  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 53  | THR  |
| 1   | L     | 84  | GLN  |
| 1   | L     | 88  | VAL  |
| 1   | L     | 98  | SER  |
| 1   | L     | 104 | THR  |
| 1   | L     | 110 | THR  |
| 1   | L     | 115 | ARG  |
| 1   | L     | 174 | GLU  |
| 1   | L     | 184 | ARG  |
| 1   | L     | 192 | LEU  |
| 1   | L     | 197 | LEU  |
| 1   | L     | 206 | TRP  |
| 1   | L     | 219 | SER  |
| 1   | L     | 244 | ARG  |
| 1   | L     | 260 | THR  |
| 1   | L     | 283 | CYS  |
| 1   | L     | 286 | LYS  |
| 1   | M     | 14  | VAL  |
| 1   | M     | 15  | ASP  |
| 1   | M     | 35  | ASP  |
| 1   | M     | 39  | THR  |
| 1   | M     | 57  | THR  |
| 1   | M     | 68  | ASP  |
| 1   | M     | 90  | MET  |
| 1   | M     | 98  | SER  |
| 1   | M     | 104 | THR  |
| 1   | M     | 110 | THR  |
| 1   | M     | 115 | ARG  |
| 1   | M     | 118 | LEU  |
| 1   | M     | 142 | THR  |
| 1   | M     | 149 | ILE  |
| 1   | M     | 150 | THR  |
| 1   | M     | 157 | VAL  |
| 1   | M     | 159 | ARG  |
| 1   | M     | 186 | SER  |
| 1   | M     | 191 | THR  |
| 1   | M     | 192 | LEU  |
| 1   | M     | 202 | LEU  |
| 1   | M     | 210 | ARG  |
| 1   | M     | 212 | LYS  |
| 1   | M     | 294 | GLU  |
| 1   | N     | 13  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 15  | ASP  |
| 1   | N     | 16  | VAL  |
| 1   | N     | 17  | VAL  |
| 1   | N     | 22  | GLU  |
| 1   | N     | 34  | VAL  |
| 1   | N     | 39  | THR  |
| 1   | N     | 44  | MET  |
| 1   | N     | 47  | VAL  |
| 1   | N     | 52  | ARG  |
| 1   | N     | 57  | THR  |
| 1   | N     | 90  | MET  |
| 1   | N     | 100 | VAL  |
| 1   | N     | 118 | LEU  |
| 1   | N     | 122 | VAL  |
| 1   | N     | 150 | THR  |
| 1   | N     | 154 | LYS  |
| 1   | N     | 157 | VAL  |
| 1   | N     | 159 | ARG  |
| 1   | N     | 191 | THR  |
| 1   | N     | 197 | LEU  |
| 1   | N     | 202 | LEU  |
| 1   | N     | 210 | ARG  |
| 1   | N     | 211 | ILE  |
| 1   | N     | 212 | LYS  |
| 1   | N     | 226 | SER  |
| 1   | N     | 247 | ILE  |
| 1   | N     | 260 | THR  |
| 1   | N     | 271 | LEU  |
| 1   | O     | 13  | GLU  |
| 1   | O     | 15  | ASP  |
| 1   | O     | 32  | THR  |
| 1   | O     | 39  | THR  |
| 1   | O     | 40  | ILE  |
| 1   | O     | 55  | THR  |
| 1   | O     | 62  | SER  |
| 1   | O     | 66  | THR  |
| 1   | O     | 70  | PHE  |
| 1   | O     | 90  | MET  |
| 1   | O     | 93  | THR  |
| 1   | O     | 98  | SER  |
| 1   | O     | 104 | THR  |
| 1   | O     | 110 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 115 | ARG  |
| 1   | O     | 117 | GLN  |
| 1   | O     | 186 | SER  |
| 1   | O     | 191 | THR  |
| 1   | O     | 214 | LEU  |
| 1   | O     | 258 | VAL  |
| 1   | O     | 264 | LYS  |
| 1   | O     | 272 | CYS  |
| 1   | O     | 284 | LEU  |
| 1   | O     | 286 | LYS  |
| 1   | O     | 294 | GLU  |
| 1   | P     | 14  | VAL  |
| 1   | P     | 16  | VAL  |
| 1   | P     | 34  | VAL  |
| 1   | P     | 37  | LYS  |
| 1   | P     | 39  | THR  |
| 1   | P     | 51  | THR  |
| 1   | P     | 54  | VAL  |
| 1   | P     | 57  | THR  |
| 1   | P     | 62  | SER  |
| 1   | P     | 93  | THR  |
| 1   | P     | 98  | SER  |
| 1   | P     | 104 | THR  |
| 1   | P     | 115 | ARG  |
| 1   | P     | 118 | LEU  |
| 1   | P     | 142 | THR  |
| 1   | P     | 143 | GLN  |
| 1   | P     | 147 | GLN  |
| 1   | P     | 149 | ILE  |
| 1   | P     | 157 | VAL  |
| 1   | P     | 159 | ARG  |
| 1   | P     | 180 | THR  |
| 1   | P     | 186 | SER  |
| 1   | P     | 191 | THR  |
| 1   | P     | 192 | LEU  |
| 1   | P     | 196 | LYS  |
| 1   | P     | 197 | LEU  |
| 1   | P     | 211 | ILE  |
| 1   | P     | 212 | LYS  |
| 1   | P     | 229 | GLN  |
| 1   | P     | 244 | ARG  |
| 1   | P     | 272 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 286 | LYS  |
| 1   | P     | 292 | ILE  |
| 1   | R     | 14  | VAL  |
| 1   | R     | 15  | ASP  |
| 1   | R     | 29  | ARG  |
| 1   | R     | 35  | ASP  |
| 1   | R     | 37  | LYS  |
| 1   | R     | 39  | THR  |
| 1   | R     | 65  | SER  |
| 1   | R     | 86  | SER  |
| 1   | R     | 90  | MET  |
| 1   | R     | 92  | GLN  |
| 1   | R     | 98  | SER  |
| 1   | R     | 99  | LYS  |
| 1   | R     | 115 | ARG  |
| 1   | R     | 157 | VAL  |
| 1   | R     | 165 | LYS  |
| 1   | R     | 171 | LYS  |
| 1   | R     | 191 | THR  |
| 1   | R     | 196 | LYS  |
| 1   | R     | 197 | LEU  |
| 1   | R     | 211 | ILE  |
| 1   | R     | 212 | LYS  |
| 1   | R     | 219 | SER  |
| 1   | R     | 244 | ARG  |
| 1   | R     | 284 | LEU  |
| 1   | R     | 286 | LYS  |
| 1   | S     | 15  | ASP  |
| 1   | S     | 16  | VAL  |
| 1   | S     | 17  | VAL  |
| 1   | S     | 37  | LYS  |
| 1   | S     | 39  | THR  |
| 1   | S     | 90  | MET  |
| 1   | S     | 93  | THR  |
| 1   | S     | 95  | VAL  |
| 1   | S     | 98  | SER  |
| 1   | S     | 110 | THR  |
| 1   | S     | 115 | ARG  |
| 1   | S     | 118 | LEU  |
| 1   | S     | 149 | ILE  |
| 1   | S     | 150 | THR  |
| 1   | S     | 152 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S     | 186 | SER  |
| 1   | S     | 191 | THR  |
| 1   | S     | 197 | LEU  |
| 1   | S     | 202 | LEU  |
| 1   | S     | 210 | ARG  |
| 1   | S     | 232 | ILE  |
| 1   | S     | 283 | CYS  |
| 1   | S     | 284 | LEU  |
| 1   | S     | 287 | ARG  |
| 1   | S     | 290 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 36  | GLN  |
| 1   | A     | 48  | ASN  |
| 1   | A     | 58  | HIS  |
| 1   | A     | 92  | GLN  |
| 1   | B     | 36  | GLN  |
| 1   | B     | 46  | ASN  |
| 1   | B     | 48  | ASN  |
| 1   | C     | 48  | ASN  |
| 1   | C     | 92  | GLN  |
| 1   | C     | 194 | HIS  |
| 1   | C     | 240 | ASN  |
| 1   | D     | 11  | GLN  |
| 1   | D     | 36  | GLN  |
| 1   | D     | 48  | ASN  |
| 1   | D     | 58  | HIS  |
| 1   | D     | 117 | GLN  |
| 1   | D     | 236 | GLN  |
| 1   | E     | 11  | GLN  |
| 1   | E     | 36  | GLN  |
| 1   | E     | 46  | ASN  |
| 1   | E     | 48  | ASN  |
| 1   | E     | 92  | GLN  |
| 1   | E     | 194 | HIS  |
| 1   | E     | 229 | GLN  |
| 1   | F     | 36  | GLN  |
| 1   | F     | 117 | GLN  |
| 1   | F     | 147 | GLN  |
| 1   | G     | 28  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 36  | GLN  |
| 1   | G     | 103 | HIS  |
| 1   | G     | 172 | HIS  |
| 1   | G     | 240 | ASN  |
| 1   | H     | 36  | GLN  |
| 1   | H     | 48  | ASN  |
| 1   | H     | 58  | HIS  |
| 1   | H     | 84  | GLN  |
| 1   | H     | 172 | HIS  |
| 1   | H     | 194 | HIS  |
| 1   | I     | 48  | ASN  |
| 1   | I     | 92  | GLN  |
| 1   | I     | 160 | GLN  |
| 1   | I     | 229 | GLN  |
| 1   | I     | 240 | ASN  |
| 1   | J     | 36  | GLN  |
| 1   | J     | 240 | ASN  |
| 1   | K     | 48  | ASN  |
| 1   | K     | 58  | HIS  |
| 1   | K     | 84  | GLN  |
| 1   | K     | 117 | GLN  |
| 1   | K     | 143 | GLN  |
| 1   | K     | 194 | HIS  |
| 1   | L     | 36  | GLN  |
| 1   | L     | 48  | ASN  |
| 1   | L     | 84  | GLN  |
| 1   | L     | 87  | GLN  |
| 1   | L     | 119 | ASN  |
| 1   | M     | 36  | GLN  |
| 1   | M     | 58  | HIS  |
| 1   | M     | 84  | GLN  |
| 1   | M     | 92  | GLN  |
| 1   | M     | 172 | HIS  |
| 1   | M     | 240 | ASN  |
| 1   | N     | 87  | GLN  |
| 1   | N     | 117 | GLN  |
| 1   | N     | 172 | HIS  |
| 1   | N     | 236 | GLN  |
| 1   | O     | 87  | GLN  |
| 1   | P     | 28  | ASN  |
| 1   | P     | 87  | GLN  |
| 1   | P     | 117 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 160 | GLN  |
| 1   | P     | 172 | HIS  |
| 1   | P     | 229 | GLN  |
| 1   | R     | 48  | ASN  |
| 1   | R     | 84  | GLN  |
| 1   | R     | 92  | GLN  |
| 1   | R     | 172 | HIS  |
| 1   | R     | 243 | GLN  |
| 1   | S     | 11  | GLN  |
| 1   | S     | 58  | HIS  |
| 1   | S     | 84  | GLN  |
| 1   | S     | 236 | GLN  |
| 1   | S     | 240 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 14 are monoatomic - leaving 22 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 | $\# Z  > 2$ |
| 2   | MBO  | P     | 302 | 1    | 7,10,10      | 1.04 | 0           | 11,13,13    | 0.88 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | MBO  | H     | 301 | 1    | 7,10,10      | 1.01 | 0        | 11,13,13    | 1.07 | 0        |
| 2   | MBO  | M     | 301 | 1    | 7,10,10      | 0.93 | 0        | 11,13,13    | 1.14 | 0        |
| 2   | MBO  | D     | 301 | 1    | 7,10,10      | 0.90 | 0        | 11,13,13    | 1.20 | 1 (9%)   |
| 2   | MBO  | B     | 302 | 1    | 7,10,10      | 0.98 | 0        | 11,13,13    | 0.96 | 0        |
| 2   | MBO  | O     | 301 | 1    | 7,10,10      | 1.03 | 0        | 11,13,13    | 1.14 | 0        |
| 2   | MBO  | I     | 302 | 1    | 7,10,10      | 1.06 | 0        | 11,13,13    | 1.05 | 0        |
| 2   | MBO  | M     | 302 | 1    | 7,10,10      | 0.99 | 0        | 11,13,13    | 1.50 | 1 (9%)   |
| 2   | MBO  | C     | 301 | 1    | 7,10,10      | 1.00 | 0        | 11,13,13    | 0.80 | 0        |
| 2   | MBO  | B     | 301 | 1    | 7,10,10      | 1.02 | 0        | 11,13,13    | 1.10 | 0        |
| 2   | MBO  | L     | 302 | 1    | 7,10,10      | 1.01 | 0        | 11,13,13    | 0.96 | 0        |
| 2   | MBO  | G     | 301 | 1    | 7,10,10      | 0.96 | 0        | 11,13,13    | 1.03 | 0        |
| 2   | MBO  | F     | 302 | 1    | 7,10,10      | 1.01 | 0        | 11,13,13    | 1.20 | 0        |
| 2   | MBO  | A     | 302 | 1    | 7,10,10      | 1.19 | 0        | 11,13,13    | 1.01 | 0        |
| 2   | MBO  | R     | 301 | 1    | 7,10,10      | 0.97 | 0        | 11,13,13    | 0.98 | 0        |
| 2   | MBO  | S     | 301 | 1    | 7,10,10      | 0.85 | 0        | 11,13,13    | 1.16 | 0        |
| 2   | MBO  | A     | 301 | 1    | 7,10,10      | 1.05 | 0        | 11,13,13    | 0.90 | 0        |
| 2   | MBO  | L     | 301 | 1    | 7,10,10      | 0.95 | 0        | 11,13,13    | 0.89 | 0        |
| 2   | MBO  | K     | 301 | 1    | 7,10,10      | 1.01 | 0        | 11,13,13    | 1.26 | 0        |
| 2   | MBO  | K     | 302 | 1    | 7,10,10      | 0.94 | 0        | 11,13,13    | 0.96 | 0        |
| 2   | MBO  | E     | 301 | 1    | 7,10,10      | 0.98 | 0        | 11,13,13    | 1.01 | 0        |
| 2   | MBO  | H     | 302 | 1    | 7,10,10      | 1.03 | 0        | 11,13,13    | 1.19 | 1 (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   |
|-----|------|-------|-----|------|---------|----------|---------|
| 2   | MBO  | P     | 302 | 1    | -       | 0/4/4/4  | 0/1/1/1 |
| 2   | MBO  | H     | 301 | 1    | -       | 4/4/4/4  | 0/1/1/1 |
| 2   | MBO  | M     | 301 | 1    | -       | 4/4/4/4  | 0/1/1/1 |
| 2   | MBO  | D     | 301 | 1    | -       | 4/4/4/4  | 0/1/1/1 |
| 2   | MBO  | B     | 302 | 1    | -       | 4/4/4/4  | 0/1/1/1 |
| 2   | MBO  | O     | 301 | 1    | -       | 4/4/4/4  | 0/1/1/1 |
| 2   | MBO  | I     | 302 | 1    | -       | 4/4/4/4  | 0/1/1/1 |
| 2   | MBO  | M     | 302 | 1    | -       | 4/4/4/4  | 0/1/1/1 |
| 2   | MBO  | C     | 301 | 1    | -       | 4/4/4/4  | 0/1/1/1 |
| 2   | MBO  | B     | 301 | 1    | -       | 4/4/4/4  | 0/1/1/1 |
| 2   | MBO  | L     | 302 | 1    | -       | 4/4/4/4  | 0/1/1/1 |
| 2   | MBO  | G     | 301 | 1    | -       | 0/4/4/4  | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 2   | MBO  | F     | 302 | 1    | -       | 4/4/4/4  | 0/1/1/1 |
| 2   | MBO  | A     | 302 | 1    | -       | 4/4/4/4  | 0/1/1/1 |
| 2   | MBO  | R     | 301 | 1    | -       | 4/4/4/4  | 0/1/1/1 |
| 2   | MBO  | S     | 301 | 1    | -       | 4/4/4/4  | 0/1/1/1 |
| 2   | MBO  | A     | 301 | 1    | -       | 4/4/4/4  | 0/1/1/1 |
| 2   | MBO  | L     | 301 | 1    | -       | 0/4/4/4  | 0/1/1/1 |
| 2   | MBO  | K     | 301 | 1    | -       | 4/4/4/4  | 0/1/1/1 |
| 2   | MBO  | K     | 302 | 1    | -       | 4/4/4/4  | 0/1/1/1 |
| 2   | MBO  | E     | 301 | 1    | -       | 0/4/4/4  | 0/1/1/1 |
| 2   | MBO  | H     | 302 | 1    | -       | 4/4/4/4  | 0/1/1/1 |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | M     | 302 | MBO  | CE5-CE4-CZ  | -2.26 | 115.90      | 120.37   |
| 2   | D     | 301 | MBO  | CE5-CE4-CE3 | 2.24  | 121.41      | 118.57   |
| 2   | H     | 302 | MBO  | CE5-CE4-CE3 | 2.01  | 121.12      | 118.57   |

There are no chirality outliers.

All (72) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | A     | 302 | MBO  | CE5-CE4-CZ-OZ2 |
| 2   | C     | 301 | MBO  | CE5-CE4-CZ-OZ2 |
| 2   | M     | 301 | MBO  | CE5-CE4-CZ-OZ2 |
| 2   | A     | 302 | MBO  | CE3-CE4-CZ-OZ1 |
| 2   | B     | 302 | MBO  | CE5-CE4-CZ-OZ1 |
| 2   | C     | 301 | MBO  | CE3-CE4-CZ-OZ1 |
| 2   | L     | 302 | MBO  | CE3-CE4-CZ-OZ1 |
| 2   | L     | 302 | MBO  | CE5-CE4-CZ-OZ1 |
| 2   | M     | 301 | MBO  | CE3-CE4-CZ-OZ1 |
| 2   | R     | 301 | MBO  | CE3-CE4-CZ-OZ1 |
| 2   | R     | 301 | MBO  | CE5-CE4-CZ-OZ1 |
| 2   | A     | 302 | MBO  | CE3-CE4-CZ-OZ2 |
| 2   | C     | 301 | MBO  | CE3-CE4-CZ-OZ2 |
| 2   | D     | 301 | MBO  | CE3-CE4-CZ-OZ2 |
| 2   | F     | 302 | MBO  | CE5-CE4-CZ-OZ2 |
| 2   | H     | 302 | MBO  | CE3-CE4-CZ-OZ2 |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | L     | 302 | MBO  | CE3-CE4-CZ-OZ2 |
| 2   | L     | 302 | MBO  | CE5-CE4-CZ-OZ2 |
| 2   | M     | 301 | MBO  | CE3-CE4-CZ-OZ2 |
| 2   | R     | 301 | MBO  | CE3-CE4-CZ-OZ2 |
| 2   | R     | 301 | MBO  | CE5-CE4-CZ-OZ2 |
| 2   | A     | 302 | MBO  | CE5-CE4-CZ-OZ1 |
| 2   | B     | 301 | MBO  | CE5-CE4-CZ-OZ1 |
| 2   | C     | 301 | MBO  | CE5-CE4-CZ-OZ1 |
| 2   | D     | 301 | MBO  | CE3-CE4-CZ-OZ1 |
| 2   | D     | 301 | MBO  | CE5-CE4-CZ-OZ1 |
| 2   | F     | 302 | MBO  | CE3-CE4-CZ-OZ1 |
| 2   | F     | 302 | MBO  | CE5-CE4-CZ-OZ1 |
| 2   | H     | 302 | MBO  | CE3-CE4-CZ-OZ1 |
| 2   | H     | 302 | MBO  | CE5-CE4-CZ-OZ1 |
| 2   | M     | 301 | MBO  | CE5-CE4-CZ-OZ1 |
| 2   | O     | 301 | MBO  | CE3-CE4-CZ-OZ1 |
| 2   | S     | 301 | MBO  | CE3-CE4-CZ-OZ1 |
| 2   | B     | 302 | MBO  | CE3-CE4-CZ-OZ2 |
| 2   | H     | 302 | MBO  | CE5-CE4-CZ-OZ2 |
| 2   | O     | 301 | MBO  | CE5-CE4-CZ-OZ2 |
| 2   | B     | 301 | MBO  | CE3-CE4-CZ-OZ1 |
| 2   | O     | 301 | MBO  | CE5-CE4-CZ-OZ1 |
| 2   | S     | 301 | MBO  | CE5-CE4-CZ-OZ1 |
| 2   | B     | 301 | MBO  | CE3-CE4-CZ-OZ2 |
| 2   | F     | 302 | MBO  | CE3-CE4-CZ-OZ2 |
| 2   | B     | 302 | MBO  | CE3-CE4-CZ-OZ1 |
| 2   | S     | 301 | MBO  | CE5-CE4-CZ-OZ2 |
| 2   | K     | 301 | MBO  | CE3-CE4-CZ-OZ1 |
| 2   | K     | 301 | MBO  | CE5-CE4-CZ-OZ1 |
| 2   | M     | 302 | MBO  | CE3-CE4-CZ-OZ1 |
| 2   | M     | 302 | MBO  | CE5-CE4-CZ-OZ1 |
| 2   | B     | 302 | MBO  | CE5-CE4-CZ-OZ2 |
| 2   | D     | 301 | MBO  | CE5-CE4-CZ-OZ2 |
| 2   | K     | 301 | MBO  | CE3-CE4-CZ-OZ2 |
| 2   | M     | 302 | MBO  | CE5-CE4-CZ-OZ2 |
| 2   | O     | 301 | MBO  | CE3-CE4-CZ-OZ2 |
| 2   | B     | 301 | MBO  | CE5-CE4-CZ-OZ2 |
| 2   | M     | 302 | MBO  | CE3-CE4-CZ-OZ2 |
| 2   | S     | 301 | MBO  | CE3-CE4-CZ-OZ2 |
| 2   | K     | 301 | MBO  | CE5-CE4-CZ-OZ2 |
| 2   | A     | 301 | MBO  | CE3-CE4-CZ-OZ2 |
| 2   | A     | 301 | MBO  | CE3-CE4-CZ-OZ1 |

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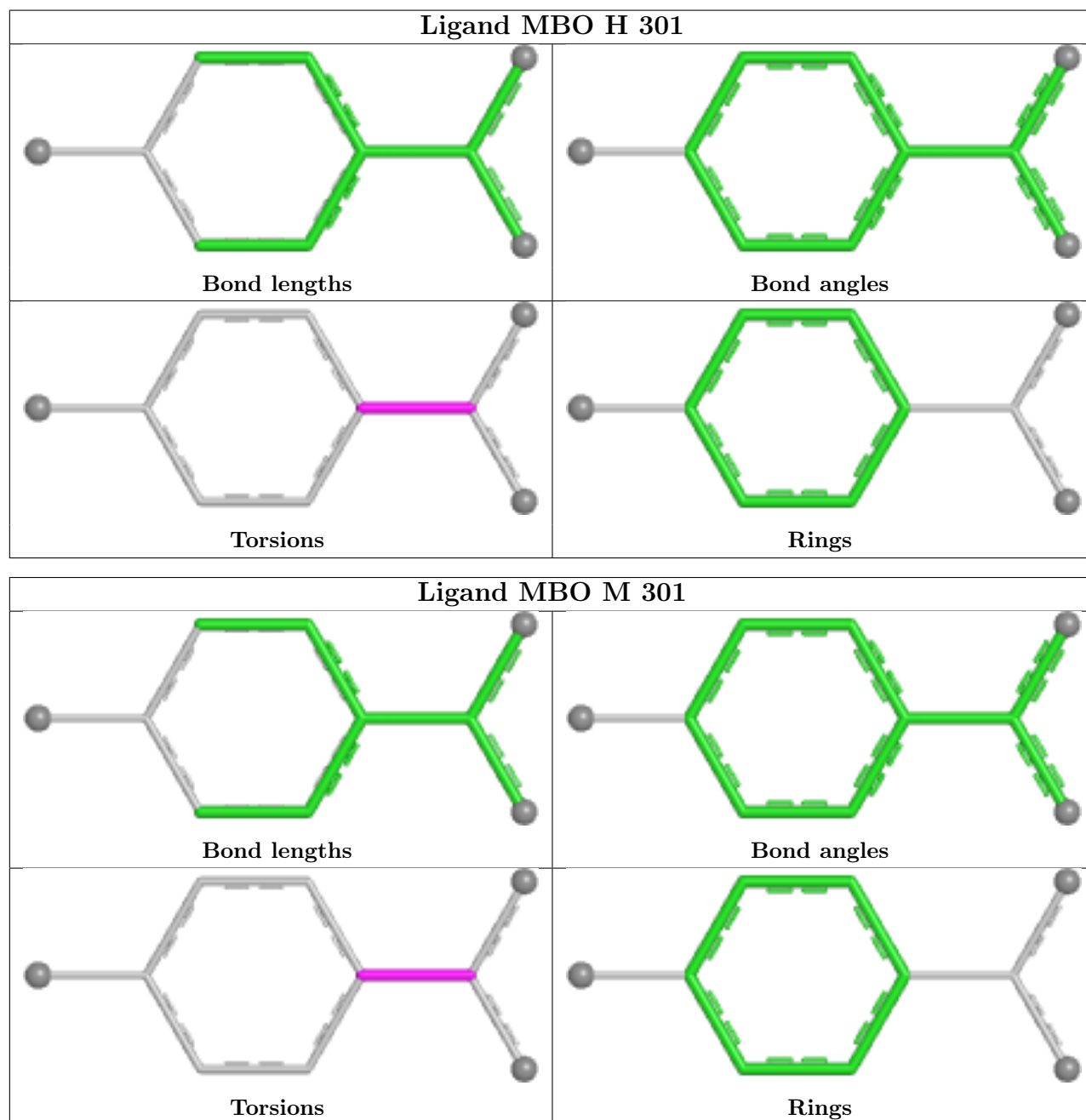
| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | A     | 301 | MBO  | CE5-CE4-CZ-OZ2 |
| 2   | A     | 301 | MBO  | CE5-CE4-CZ-OZ1 |
| 2   | H     | 301 | MBO  | CE5-CE4-CZ-OZ2 |
| 2   | H     | 301 | MBO  | CE5-CE4-CZ-OZ1 |
| 2   | H     | 301 | MBO  | CE3-CE4-CZ-OZ1 |
| 2   | H     | 301 | MBO  | CE3-CE4-CZ-OZ2 |
| 2   | I     | 302 | MBO  | CE3-CE4-CZ-OZ1 |
| 2   | I     | 302 | MBO  | CE5-CE4-CZ-OZ1 |
| 2   | I     | 302 | MBO  | CE3-CE4-CZ-OZ2 |
| 2   | I     | 302 | MBO  | CE5-CE4-CZ-OZ2 |
| 2   | K     | 302 | MBO  | CE3-CE4-CZ-OZ2 |
| 2   | K     | 302 | MBO  | CE3-CE4-CZ-OZ1 |
| 2   | K     | 302 | MBO  | CE5-CE4-CZ-OZ2 |
| 2   | K     | 302 | MBO  | CE5-CE4-CZ-OZ1 |

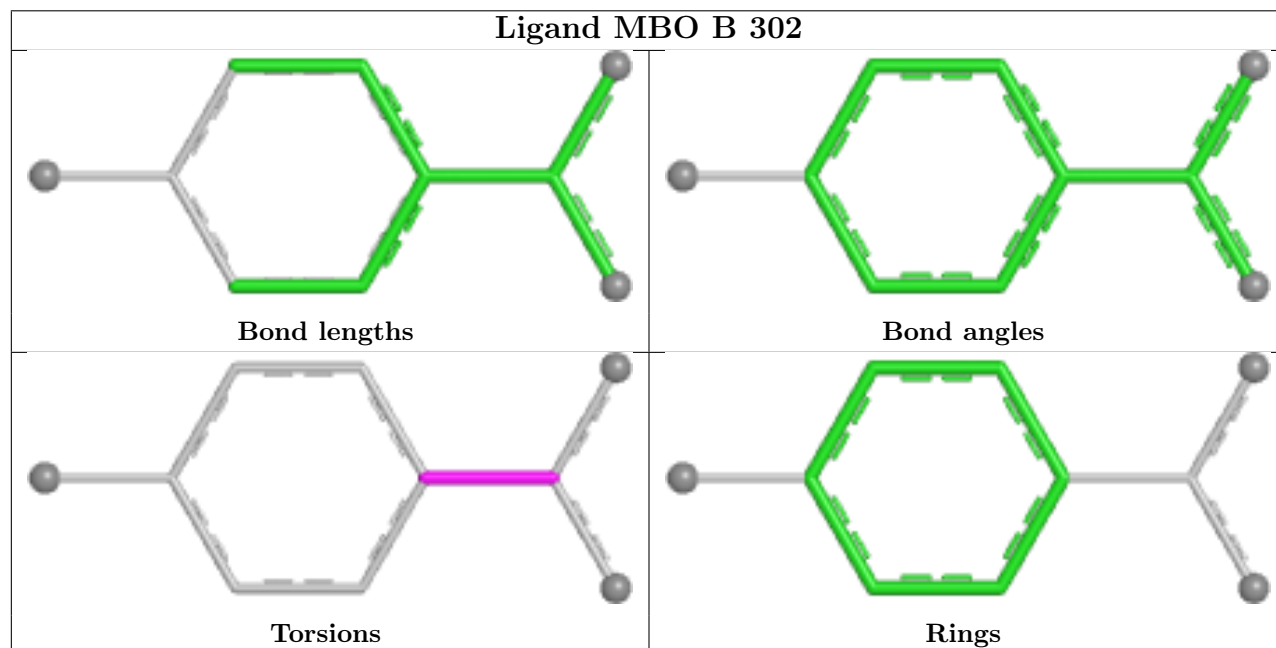
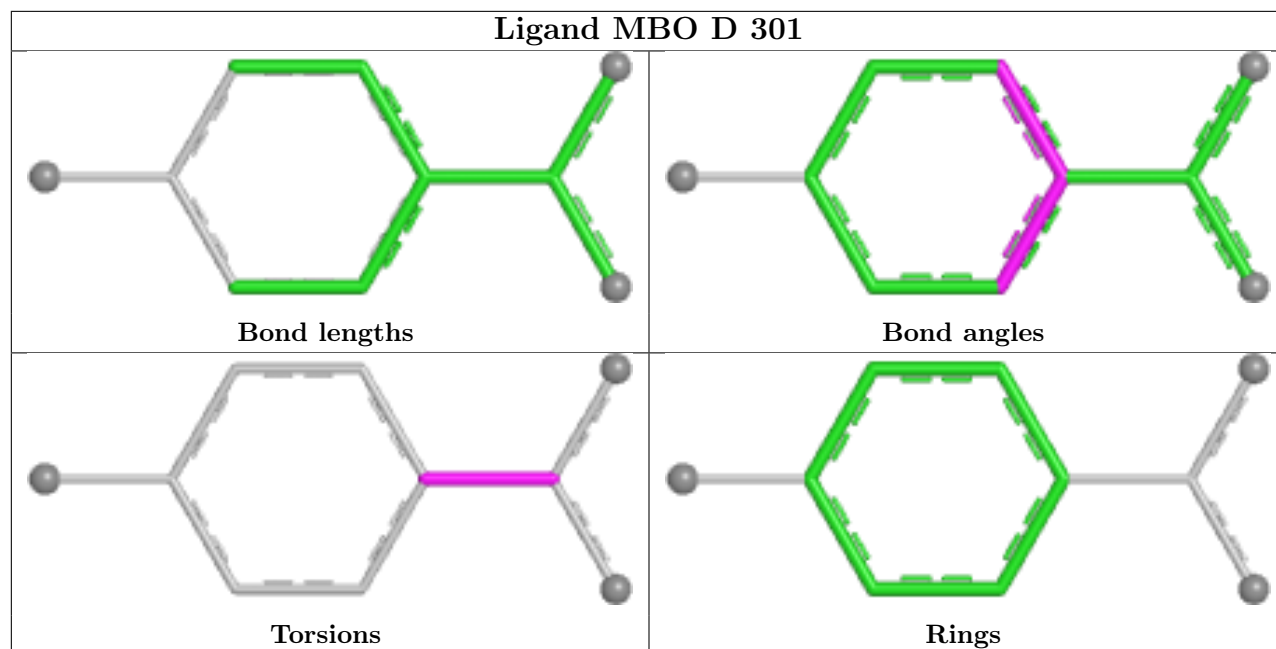
There are no ring outliers.

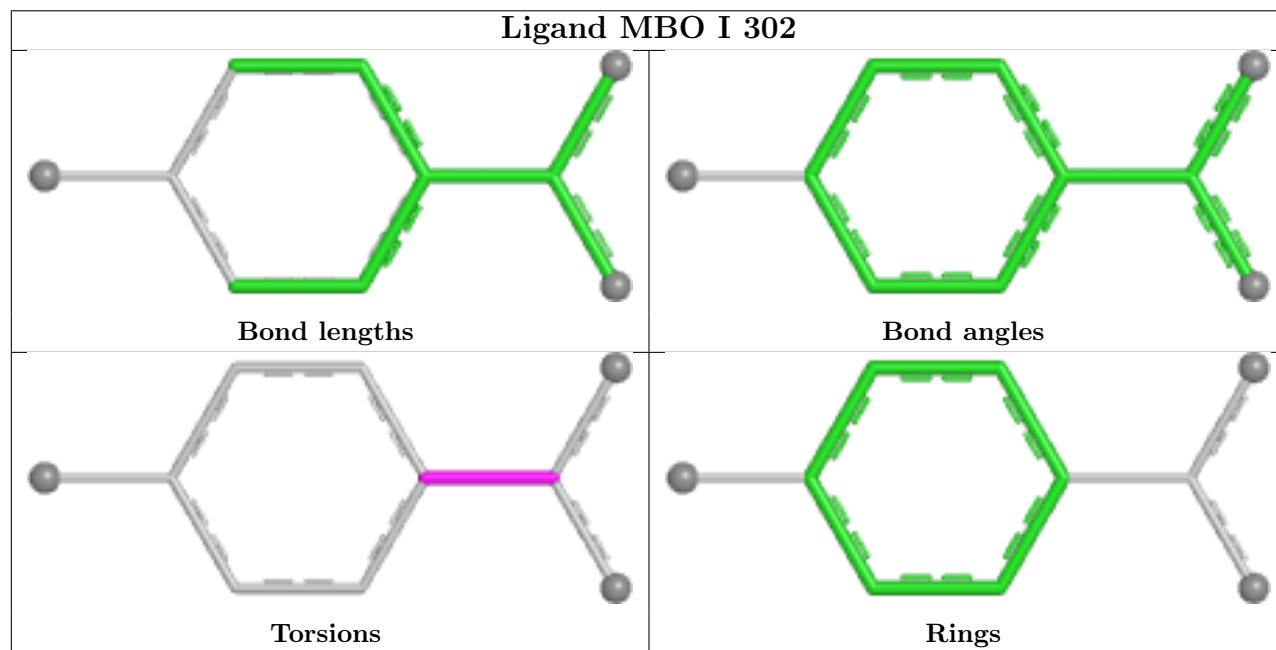
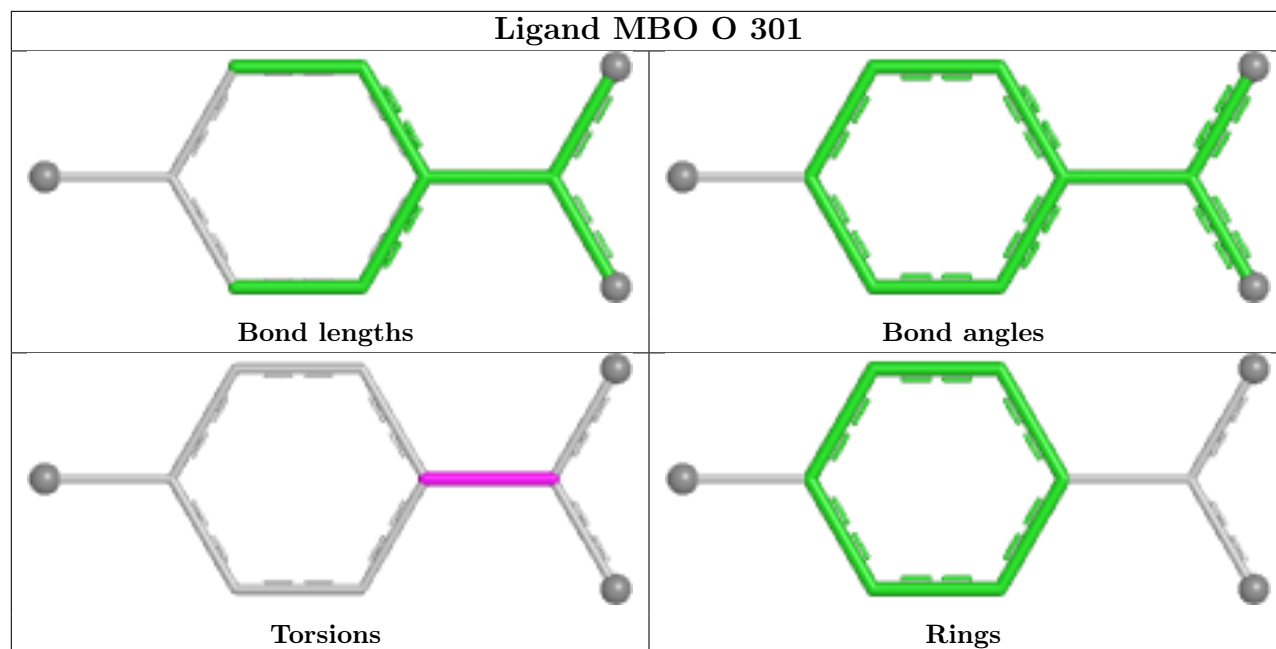
22 monomers are involved in 253 short contacts:

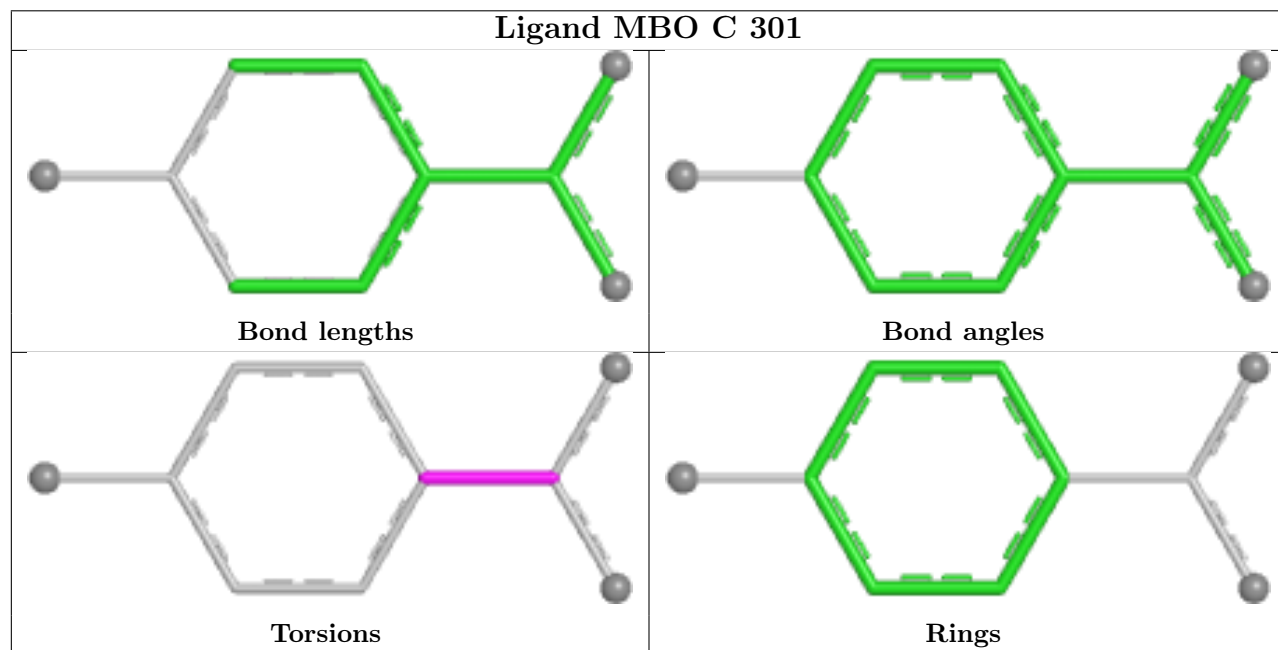
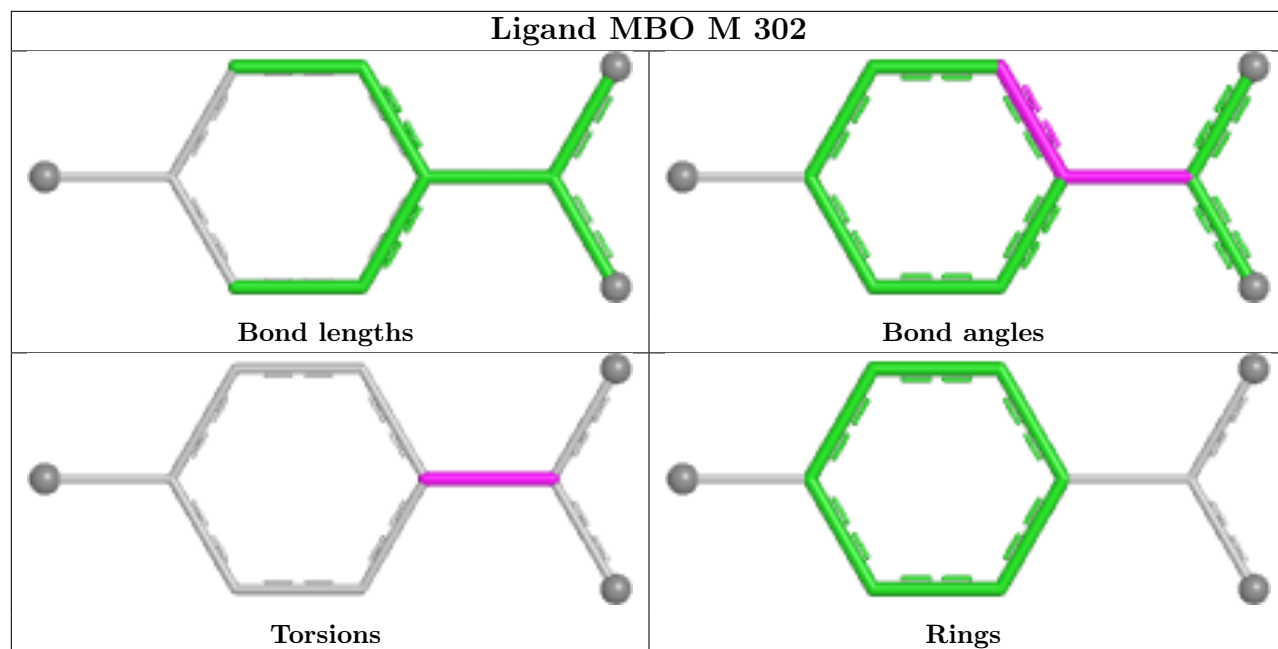
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | P     | 302 | MBO  | 20      | 0            |
| 2   | H     | 301 | MBO  | 15      | 0            |
| 2   | M     | 301 | MBO  | 17      | 0            |
| 2   | D     | 301 | MBO  | 17      | 0            |
| 2   | B     | 302 | MBO  | 3       | 0            |
| 2   | O     | 301 | MBO  | 13      | 0            |
| 2   | I     | 302 | MBO  | 6       | 0            |
| 2   | M     | 302 | MBO  | 1       | 0            |
| 2   | C     | 301 | MBO  | 10      | 0            |
| 2   | B     | 301 | MBO  | 13      | 0            |
| 2   | L     | 302 | MBO  | 8       | 0            |
| 2   | G     | 301 | MBO  | 13      | 0            |
| 2   | F     | 302 | MBO  | 19      | 0            |
| 2   | A     | 302 | MBO  | 8       | 0            |
| 2   | R     | 301 | MBO  | 7       | 0            |
| 2   | S     | 301 | MBO  | 15      | 0            |
| 2   | A     | 301 | MBO  | 1       | 0            |
| 2   | L     | 301 | MBO  | 17      | 0            |
| 2   | K     | 301 | MBO  | 16      | 0            |
| 2   | K     | 302 | MBO  | 14      | 0            |
| 2   | E     | 301 | MBO  | 6       | 0            |
| 2   | H     | 302 | MBO  | 14      | 0            |

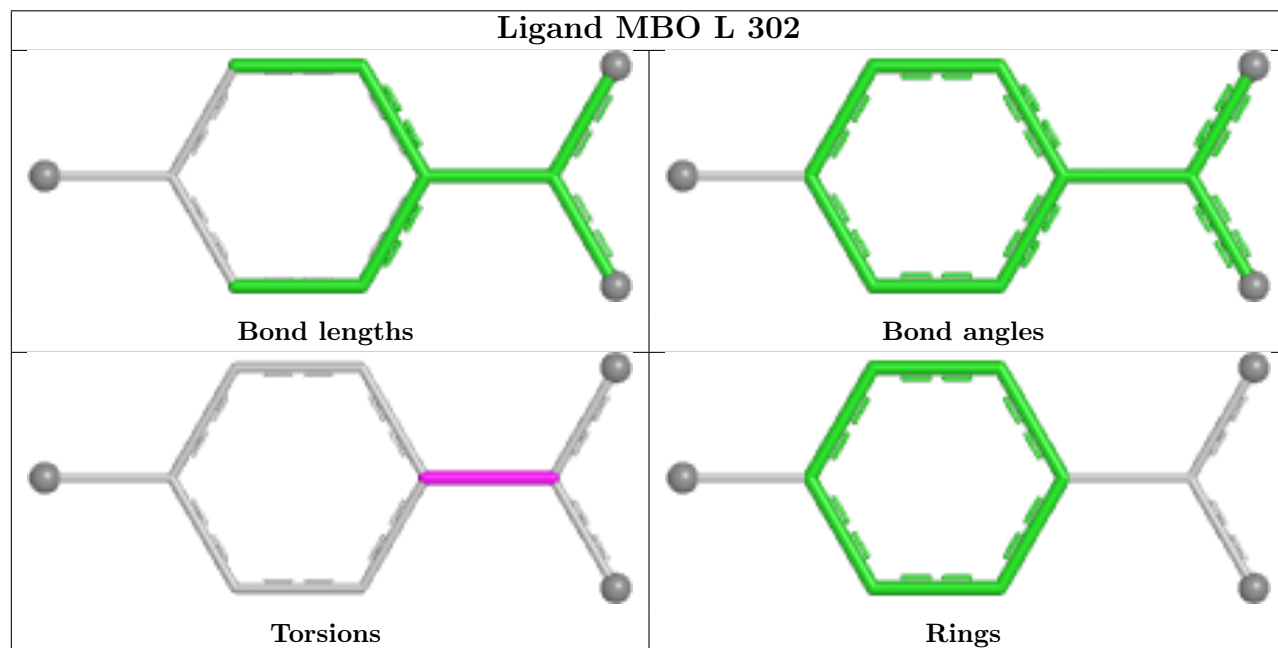
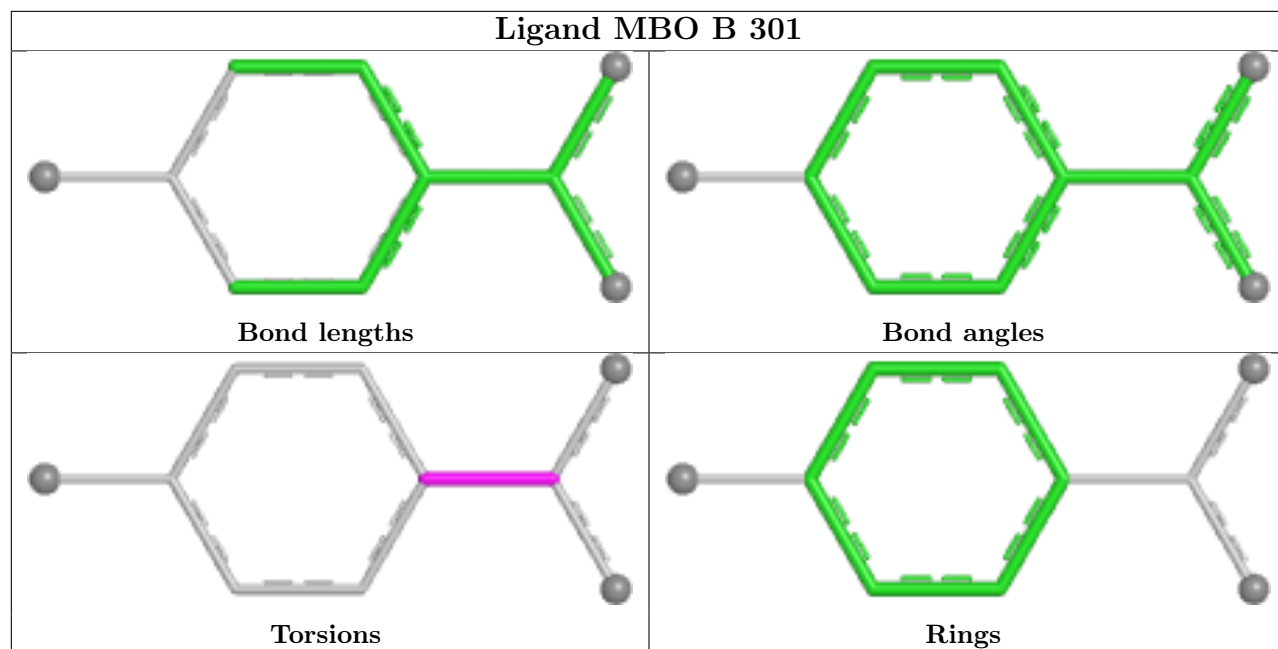
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

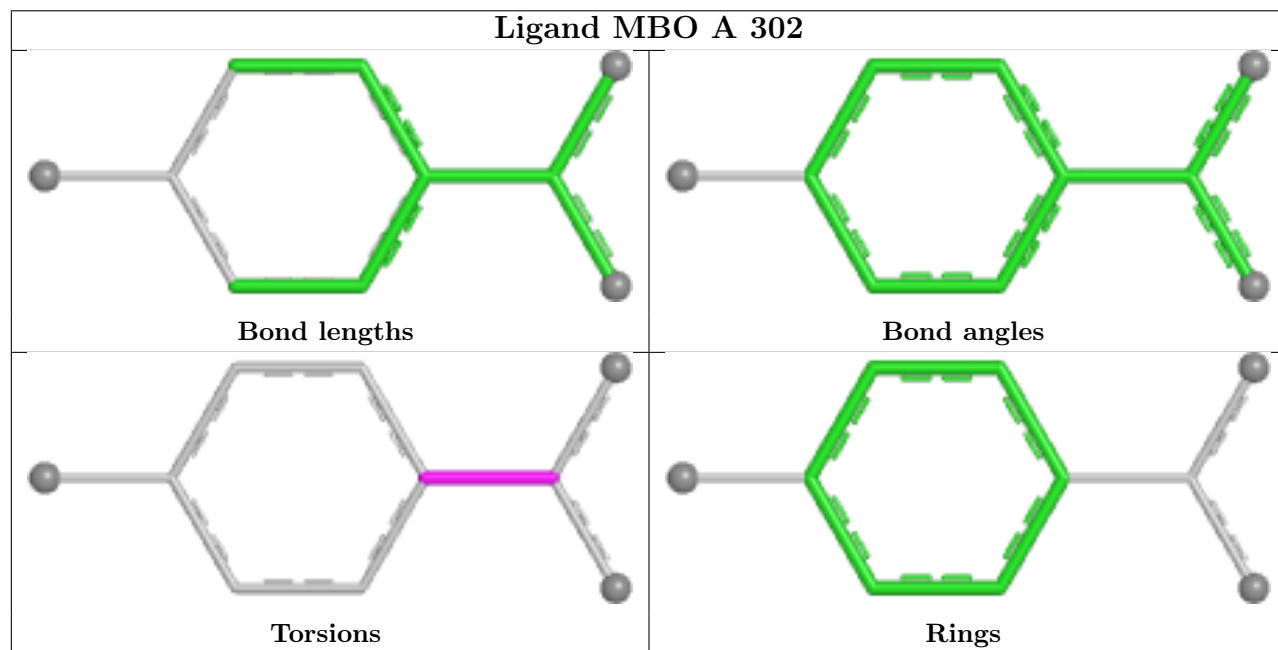
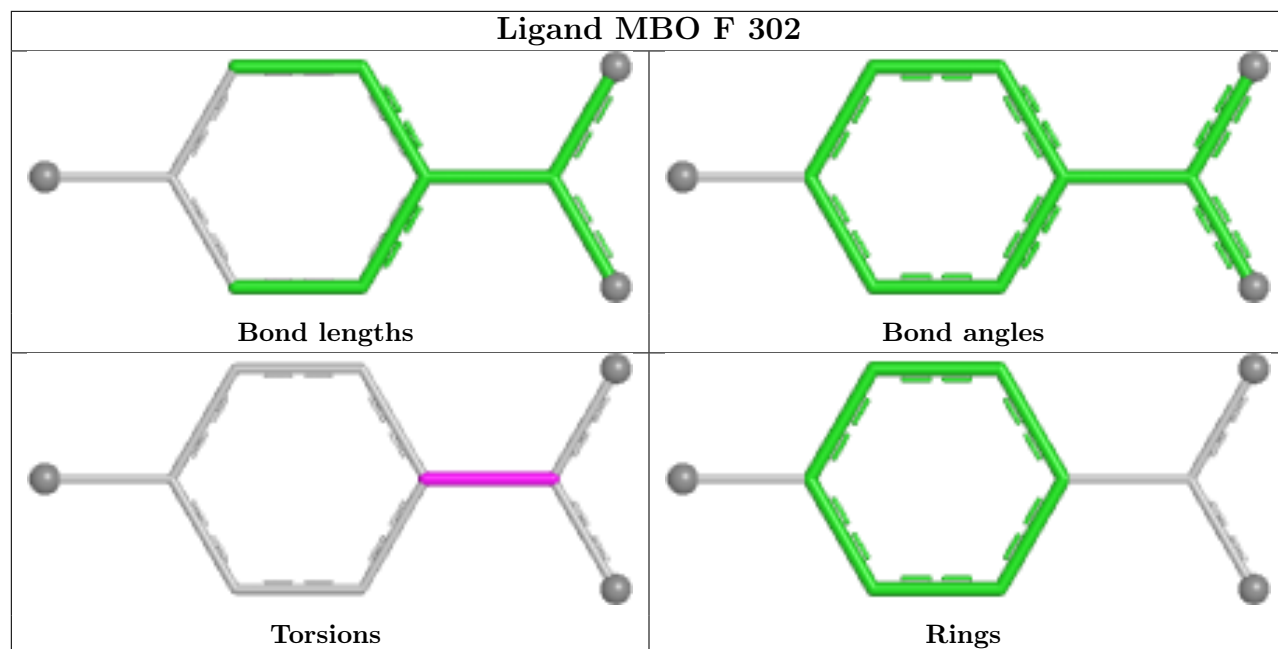


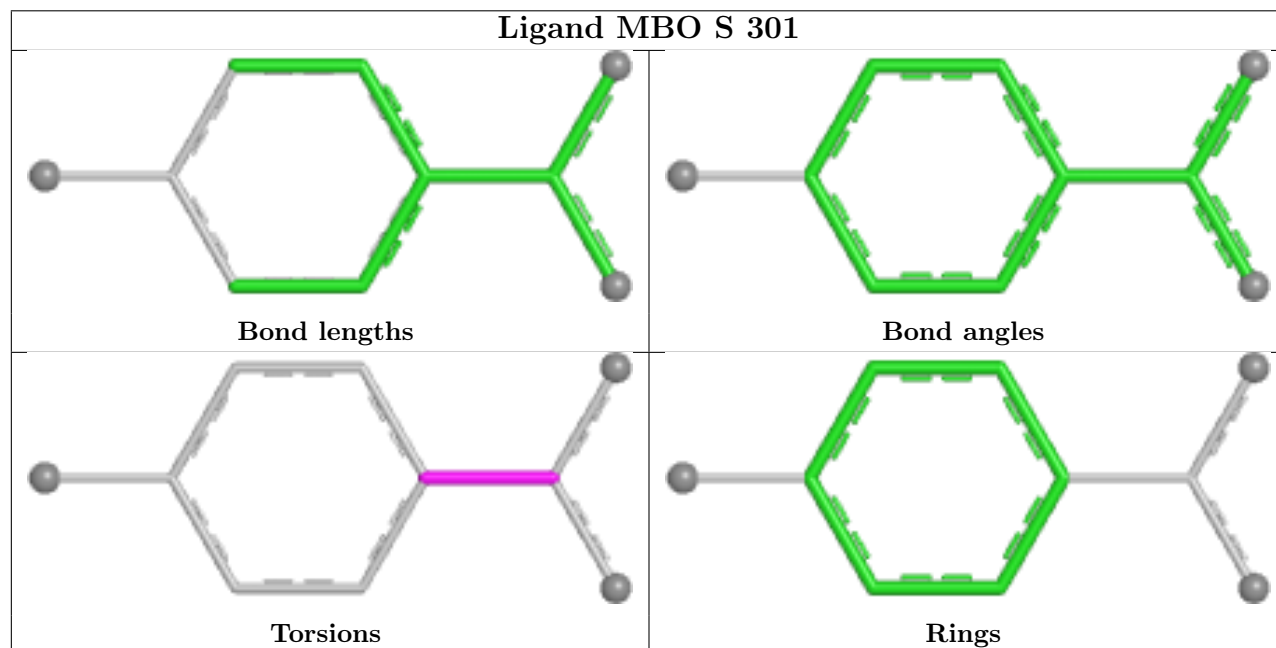
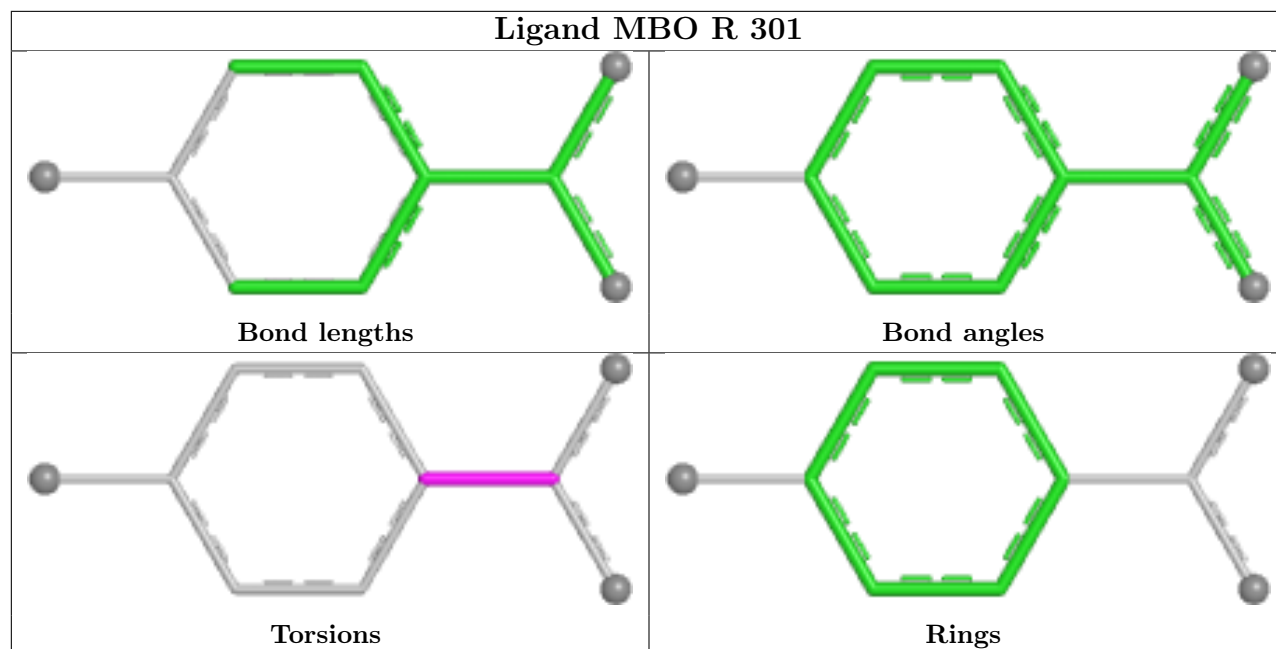


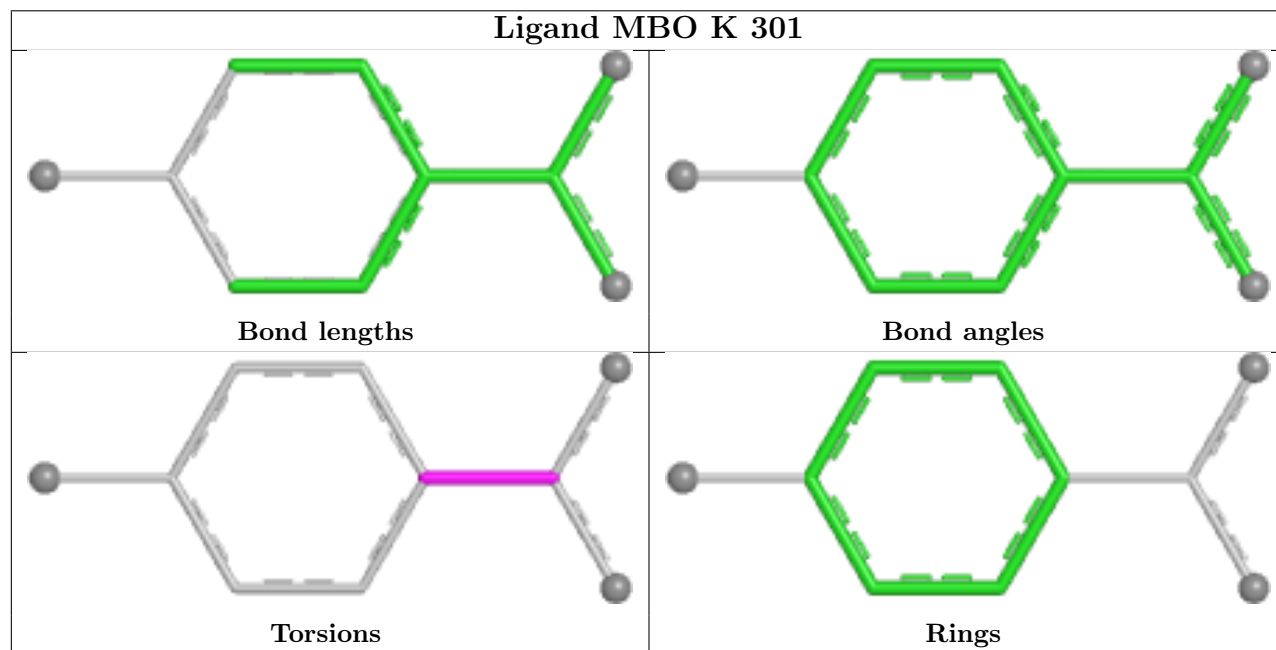
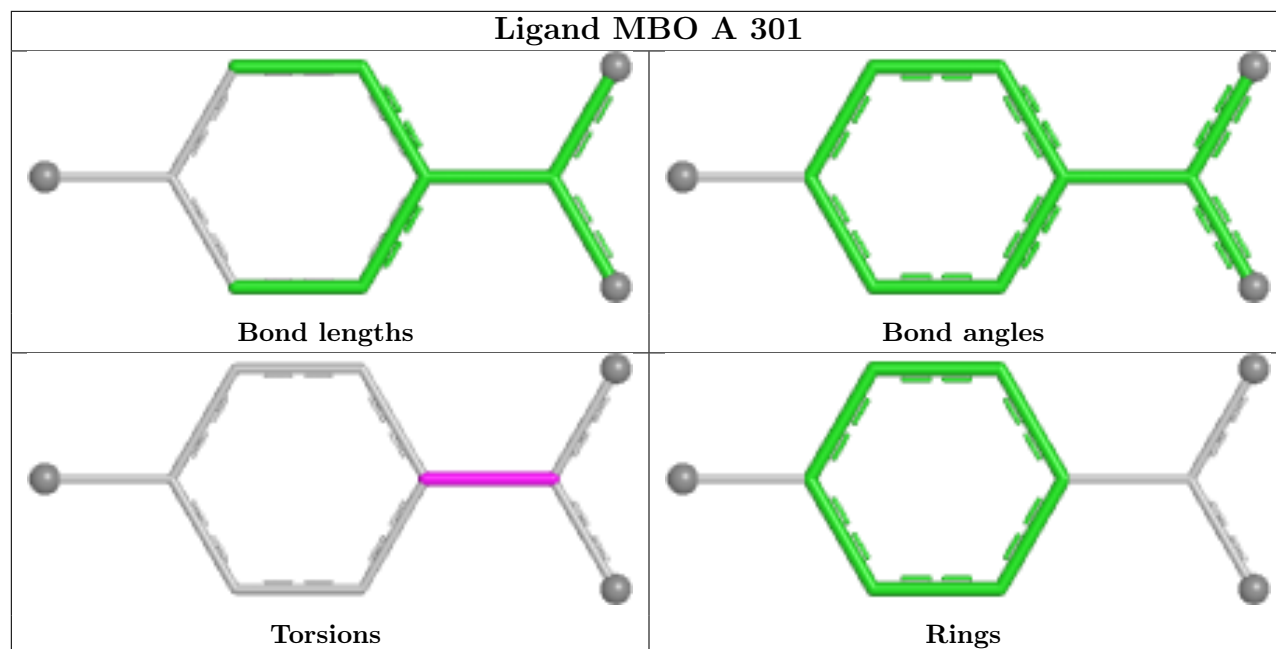


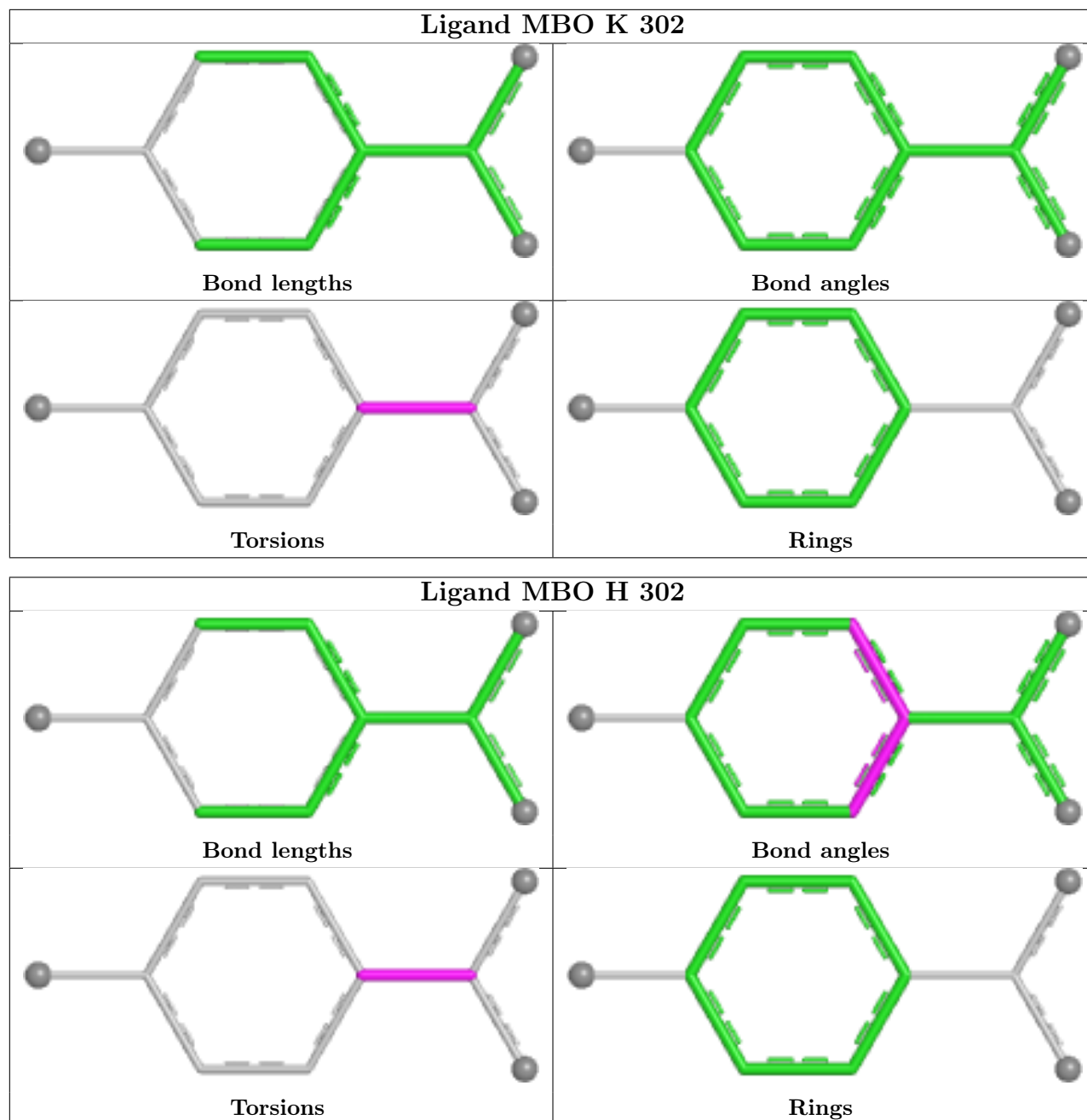












## 5.7 Other polymers [i](#)

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   | A     | 290/298 (97%)   | 0.08   | 13 (4%) 38 20  | 28, 53, 90, 141       | 0     |
| 1   | B     | 284/298 (95%)   | 0.10   | 7 (2%) 58 37   | 26, 59, 86, 126       | 0     |
| 1   | C     | 286/298 (95%)   | 0.33   | 17 (5%) 28 15  | 31, 62, 94, 134       | 0     |
| 1   | D     | 285/298 (95%)   | 0.16   | 7 (2%) 58 37   | 32, 55, 86, 132       | 0     |
| 1   | E     | 283/298 (94%)   | 0.06   | 16 (5%) 29 16  | 28, 49, 81, 111       | 0     |
| 1   | F     | 283/298 (94%)   | 0.12   | 15 (5%) 32 17  | 28, 47, 90, 124       | 0     |
| 1   | G     | 290/298 (97%)   | 0.10   | 12 (4%) 41 23  | 26, 45, 97, 145       | 0     |
| 1   | H     | 283/298 (94%)   | 0.04   | 7 (2%) 58 37   | 28, 46, 87, 112       | 0     |
| 1   | I     | 282/298 (94%)   | -0.05  | 4 (1%) 73 53   | 27, 48, 82, 111       | 0     |
| 1   | J     | 290/298 (97%)   | 0.24   | 15 (5%) 33 17  | 29, 56, 96, 141       | 0     |
| 1   | K     | 290/298 (97%)   | 0.20   | 14 (4%) 35 19  | 29, 51, 100, 155      | 0     |
| 1   | L     | 284/298 (95%)   | 0.02   | 10 (3%) 47 27  | 28, 48, 87, 114       | 0     |
| 1   | M     | 289/298 (96%)   | 0.13   | 9 (3%) 51 30   | 28, 53, 91, 145       | 0     |
| 1   | N     | 289/298 (96%)   | 0.28   | 13 (4%) 38 20  | 26, 61, 96, 161       | 0     |
| 1   | O     | 289/298 (96%)   | 0.40   | 21 (7%) 21 11  | 32, 62, 103, 155      | 0     |
| 1   | P     | 289/298 (96%)   | 0.39   | 15 (5%) 33 17  | 30, 63, 100, 151      | 0     |
| 1   | R     | 283/298 (94%)   | 0.32   | 11 (3%) 43 24  | 30, 61, 86, 115       | 0     |
| 1   | S     | 283/298 (94%)   | 0.20   | 11 (3%) 43 24  | 28, 59, 89, 121       | 0     |
| All | All   | 5152/5364 (96%) | 0.17   | 217 (4%) 40 22 | 26, 54, 92, 161       | 0     |

All (217) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 74  | SER  | 5.7  |
| 1   | O     | 72  | ILE  | 5.5  |
| 1   | F     | 75  | VAL  | 5.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 66  | THR  | 5.2  |
| 1   | N     | 72  | ILE  | 5.0  |
| 1   | R     | 239 | ASP  | 5.0  |
| 1   | I     | 239 | ASP  | 4.9  |
| 1   | F     | 239 | ASP  | 4.8  |
| 1   | K     | 236 | GLN  | 4.4  |
| 1   | J     | 206 | TRP  | 4.4  |
| 1   | P     | 206 | TRP  | 4.4  |
| 1   | I     | 206 | TRP  | 4.3  |
| 1   | A     | 221 | TYR  | 4.2  |
| 1   | A     | 72  | ILE  | 4.1  |
| 1   | C     | 8   | GLY  | 4.1  |
| 1   | R     | 237 | GLY  | 4.1  |
| 1   | P     | 72  | ILE  | 4.1  |
| 1   | F     | 206 | TRP  | 3.9  |
| 1   | E     | 55  | THR  | 3.9  |
| 1   | N     | 240 | ASN  | 3.9  |
| 1   | J     | 239 | ASP  | 3.9  |
| 1   | N     | 206 | TRP  | 3.9  |
| 1   | O     | 187 | TRP  | 3.8  |
| 1   | K     | 221 | TYR  | 3.8  |
| 1   | K     | 8   | GLY  | 3.8  |
| 1   | G     | 206 | TRP  | 3.8  |
| 1   | B     | 9   | TYR  | 3.7  |
| 1   | L     | 206 | TRP  | 3.7  |
| 1   | B     | 297 | GLY  | 3.7  |
| 1   | C     | 235 | ASP  | 3.6  |
| 1   | K     | 72  | ILE  | 3.6  |
| 1   | F     | 274 | ASP  | 3.6  |
| 1   | G     | 70  | PHE  | 3.5  |
| 1   | R     | 236 | GLN  | 3.5  |
| 1   | G     | 72  | ILE  | 3.5  |
| 1   | L     | 239 | ASP  | 3.4  |
| 1   | H     | 221 | TYR  | 3.4  |
| 1   | N     | 229 | GLN  | 3.4  |
| 1   | E     | 229 | GLN  | 3.3  |
| 1   | E     | 206 | TRP  | 3.3  |
| 1   | A     | 277 | PRO  | 3.2  |
| 1   | L     | 57  | THR  | 3.2  |
| 1   | O     | 186 | SER  | 3.2  |
| 1   | M     | 239 | ASP  | 3.2  |
| 1   | R     | 238 | THR  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 72  | ILE  | 3.2  |
| 1   | F     | 65  | SER  | 3.2  |
| 1   | R     | 243 | GLN  | 3.1  |
| 1   | E     | 65  | SER  | 3.1  |
| 1   | C     | 239 | ASP  | 3.1  |
| 1   | P     | 187 | TRP  | 3.1  |
| 1   | J     | 84  | GLN  | 3.1  |
| 1   | D     | 83  | HIS  | 3.1  |
| 1   | G     | 278 | ALA  | 3.1  |
| 1   | O     | 73  | GLY  | 3.1  |
| 1   | P     | 274 | ASP  | 3.1  |
| 1   | K     | 220 | GLY  | 3.0  |
| 1   | D     | 7   | GLU  | 3.0  |
| 1   | I     | 74  | SER  | 3.0  |
| 1   | G     | 239 | ASP  | 3.0  |
| 1   | K     | 235 | ASP  | 3.0  |
| 1   | M     | 221 | TYR  | 3.0  |
| 1   | A     | 278 | ALA  | 3.0  |
| 1   | E     | 74  | SER  | 3.0  |
| 1   | G     | 69  | ALA  | 3.0  |
| 1   | S     | 206 | TRP  | 3.0  |
| 1   | O     | 188 | PRO  | 3.0  |
| 1   | O     | 183 | SER  | 3.0  |
| 1   | F     | 84  | GLN  | 2.9  |
| 1   | C     | 243 | GLN  | 2.9  |
| 1   | O     | 218 | TYR  | 2.9  |
| 1   | N     | 239 | ASP  | 2.8  |
| 1   | B     | 206 | TRP  | 2.8  |
| 1   | G     | 68  | ASP  | 2.8  |
| 1   | R     | 206 | TRP  | 2.8  |
| 1   | H     | 60  | ILE  | 2.8  |
| 1   | F     | 62  | SER  | 2.8  |
| 1   | J     | 67  | GLY  | 2.8  |
| 1   | C     | 221 | TYR  | 2.7  |
| 1   | M     | 72  | ILE  | 2.7  |
| 1   | O     | 216 | THR  | 2.7  |
| 1   | C     | 24  | TYR  | 2.7  |
| 1   | E     | 279 | THR  | 2.7  |
| 1   | K     | 174 | GLU  | 2.7  |
| 1   | L     | 73  | GLY  | 2.7  |
| 1   | A     | 225 | TYR  | 2.7  |
| 1   | J     | 83  | HIS  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 206 | TRP  | 2.7  |
| 1   | J     | 285 | ASP  | 2.7  |
| 1   | O     | 221 | TYR  | 2.6  |
| 1   | A     | 70  | PHE  | 2.6  |
| 1   | A     | 65  | SER  | 2.6  |
| 1   | A     | 8   | GLY  | 2.6  |
| 1   | P     | 55  | THR  | 2.6  |
| 1   | O     | 217 | MET  | 2.6  |
| 1   | O     | 70  | PHE  | 2.6  |
| 1   | C     | 237 | GLY  | 2.6  |
| 1   | L     | 237 | GLY  | 2.6  |
| 1   | P     | 275 | ASP  | 2.6  |
| 1   | S     | 280 | ASN  | 2.6  |
| 1   | F     | 63  | THR  | 2.6  |
| 1   | A     | 218 | TYR  | 2.5  |
| 1   | M     | 218 | TYR  | 2.5  |
| 1   | H     | 187 | TRP  | 2.5  |
| 1   | L     | 72  | ILE  | 2.5  |
| 1   | S     | 241 | PRO  | 2.5  |
| 1   | O     | 181 | VAL  | 2.5  |
| 1   | M     | 204 | GLU  | 2.5  |
| 1   | O     | 69  | ALA  | 2.5  |
| 1   | C     | 238 | THR  | 2.5  |
| 1   | L     | 84  | GLN  | 2.5  |
| 1   | E     | 66  | THR  | 2.5  |
| 1   | N     | 238 | THR  | 2.5  |
| 1   | B     | 68  | ASP  | 2.5  |
| 1   | B     | 239 | ASP  | 2.5  |
| 1   | I     | 66  | THR  | 2.5  |
| 1   | K     | 70  | PHE  | 2.4  |
| 1   | O     | 277 | PRO  | 2.4  |
| 1   | C     | 174 | GLU  | 2.4  |
| 1   | O     | 206 | TRP  | 2.4  |
| 1   | C     | 68  | ASP  | 2.4  |
| 1   | F     | 275 | ASP  | 2.4  |
| 1   | G     | 67  | GLY  | 2.4  |
| 1   | S     | 141 | GLY  | 2.4  |
| 1   | D     | 206 | TRP  | 2.4  |
| 1   | C     | 225 | TYR  | 2.4  |
| 1   | A     | 220 | GLY  | 2.4  |
| 1   | J     | 8   | GLY  | 2.4  |
| 1   | N     | 237 | GLY  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 225 | TYR  | 2.4  |
| 1   | D     | 65  | SER  | 2.4  |
| 1   | M     | 206 | TRP  | 2.4  |
| 1   | C     | 240 | ASN  | 2.3  |
| 1   | D     | 84  | GLN  | 2.3  |
| 1   | P     | 235 | ASP  | 2.3  |
| 1   | S     | 205 | ASP  | 2.3  |
| 1   | L     | 85  | LYS  | 2.3  |
| 1   | G     | 78  | SER  | 2.3  |
| 1   | R     | 8   | GLY  | 2.3  |
| 1   | D     | 73  | GLY  | 2.3  |
| 1   | E     | 73  | GLY  | 2.3  |
| 1   | H     | 206 | TRP  | 2.3  |
| 1   | N     | 142 | THR  | 2.3  |
| 1   | F     | 58  | HIS  | 2.3  |
| 1   | P     | 280 | ASN  | 2.3  |
| 1   | K     | 84  | GLN  | 2.3  |
| 1   | J     | 71  | GLU  | 2.3  |
| 1   | S     | 66  | THR  | 2.3  |
| 1   | P     | 9   | TYR  | 2.3  |
| 1   | G     | 229 | GLN  | 2.3  |
| 1   | S     | 275 | ASP  | 2.3  |
| 1   | C     | 22  | GLU  | 2.2  |
| 1   | F     | 82  | SER  | 2.2  |
| 1   | A     | 141 | GLY  | 2.2  |
| 1   | H     | 73  | GLY  | 2.2  |
| 1   | J     | 284 | LEU  | 2.2  |
| 1   | P     | 237 | GLY  | 2.2  |
| 1   | R     | 220 | GLY  | 2.2  |
| 1   | R     | 221 | TYR  | 2.2  |
| 1   | F     | 78  | SER  | 2.2  |
| 1   | C     | 248 | ASN  | 2.2  |
| 1   | K     | 63  | THR  | 2.2  |
| 1   | P     | 69  | ALA  | 2.2  |
| 1   | P     | 285 | ASP  | 2.2  |
| 1   | H     | 66  | THR  | 2.2  |
| 1   | S     | 142 | THR  | 2.2  |
| 1   | J     | 236 | GLN  | 2.2  |
| 1   | B     | 215 | ASN  | 2.2  |
| 1   | S     | 263 | ASN  | 2.2  |
| 1   | N     | 210 | ARG  | 2.2  |
| 1   | O     | 68  | ASP  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 142 | THR  | 2.1  |
| 1   | E     | 84  | GLN  | 2.1  |
| 1   | L     | 82  | SER  | 2.1  |
| 1   | M     | 70  | PHE  | 2.1  |
| 1   | J     | 68  | ASP  | 2.1  |
| 1   | O     | 182 | VAL  | 2.1  |
| 1   | D     | 221 | TYR  | 2.1  |
| 1   | R     | 286 | LYS  | 2.1  |
| 1   | O     | 236 | GLN  | 2.1  |
| 1   | J     | 278 | ALA  | 2.1  |
| 1   | N     | 208 | GLY  | 2.1  |
| 1   | R     | 270 | GLY  | 2.1  |
| 1   | M     | 55  | THR  | 2.1  |
| 1   | S     | 229 | GLN  | 2.1  |
| 1   | M     | 237 | GLY  | 2.1  |
| 1   | P     | 276 | GLY  | 2.1  |
| 1   | E     | 280 | ASN  | 2.1  |
| 1   | C     | 289 | ASP  | 2.1  |
| 1   | G     | 275 | ASP  | 2.1  |
| 1   | O     | 285 | ASP  | 2.1  |
| 1   | N     | 287 | ARG  | 2.1  |
| 1   | K     | 9   | TYR  | 2.1  |
| 1   | C     | 278 | ALA  | 2.1  |
| 1   | A     | 236 | GLN  | 2.1  |
| 1   | S     | 73  | GLY  | 2.1  |
| 1   | J     | 82  | SER  | 2.1  |
| 1   | B     | 214 | LEU  | 2.1  |
| 1   | F     | 83  | HIS  | 2.1  |
| 1   | N     | 244 | ARG  | 2.1  |
| 1   | O     | 276 | GLY  | 2.1  |
| 1   | H     | 75  | VAL  | 2.0  |
| 1   | C     | 186 | SER  | 2.0  |
| 1   | E     | 31  | SER  | 2.0  |
| 1   | E     | 78  | SER  | 2.0  |
| 1   | E     | 217 | MET  | 2.0  |
| 1   | A     | 9   | TYR  | 2.0  |
| 1   | G     | 225 | TYR  | 2.0  |
| 1   | P     | 229 | GLN  | 2.0  |
| 1   | J     | 241 | PRO  | 2.0  |
| 1   | E     | 75  | VAL  | 2.0  |
| 1   | K     | 52  | ARG  | 2.0  |
| 1   | E     | 63  | THR  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 69  | ALA  | 2.0  |
| 1   | P     | 225 | TYR  | 2.0  |
| 1   | O     | 220 | GLY  | 2.0  |
| 1   | N     | 71  | GLU  | 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | HG   | O     | 302 | 1/1   | 0.98 | 0.04 | 88,88,88,88                | 0     |
| 2   | MBO  | H     | 302 | 10/10 | 0.99 | 0.09 | 55,71,77,78                | 0     |
| 2   | MBO  | K     | 301 | 10/10 | 0.99 | 0.08 | 63,80,84,86                | 0     |
| 2   | MBO  | M     | 302 | 10/10 | 0.99 | 0.10 | 68,75,82,83                | 0     |
| 2   | MBO  | O     | 301 | 10/10 | 0.99 | 0.08 | 78,86,97,98                | 0     |
| 2   | MBO  | P     | 302 | 10/10 | 0.99 | 0.07 | 83,95,99,99                | 0     |
| 2   | MBO  | R     | 301 | 10/10 | 0.99 | 0.07 | 79,104,113,119             | 0     |
| 3   | HG   | C     | 302 | 1/1   | 0.99 | 0.04 | 80,80,80,80                | 0     |
| 3   | HG   | E     | 302 | 1/1   | 0.99 | 0.03 | 66,66,66,66                | 0     |
| 3   | HG   | G     | 302 | 1/1   | 0.99 | 0.02 | 58,58,58,58                | 0     |
| 3   | HG   | I     | 301 | 1/1   | 0.99 | 0.05 | 67,67,67,67                | 0     |
| 3   | HG   | J     | 301 | 1/1   | 0.99 | 0.03 | 66,66,66,66                | 0     |
| 3   | HG   | J     | 302 | 1/1   | 0.99 | 0.03 | 79,79,79,79                | 0     |
| 3   | HG   | N     | 301 | 1/1   | 0.99 | 0.03 | 70,70,70,70                | 0     |
| 3   | HG   | N     | 302 | 1/1   | 0.99 | 0.04 | 78,78,78,78                | 0     |
| 2   | MBO  | C     | 301 | 10/10 | 0.99 | 0.06 | 80,96,100,101              | 0     |
| 3   | HG   | P     | 301 | 1/1   | 0.99 | 0.03 | 81,81,81,81                | 0     |
| 3   | HG   | R     | 302 | 1/1   | 0.99 | 0.03 | 83,83,83,83                | 0     |
| 3   | HG   | S     | 302 | 1/1   | 0.99 | 0.02 | 77,77,77,77                | 0     |

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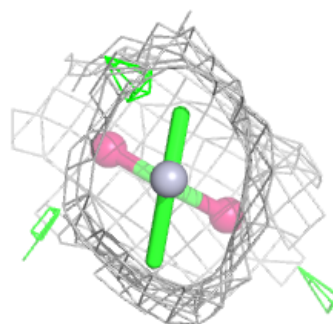
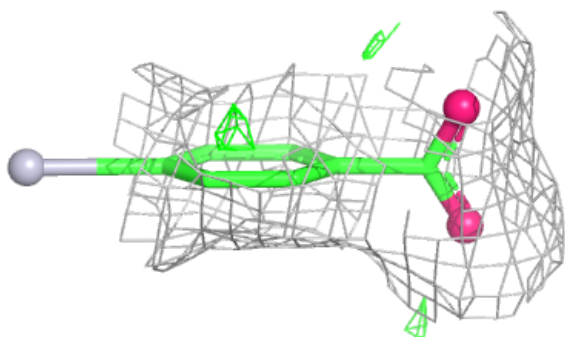
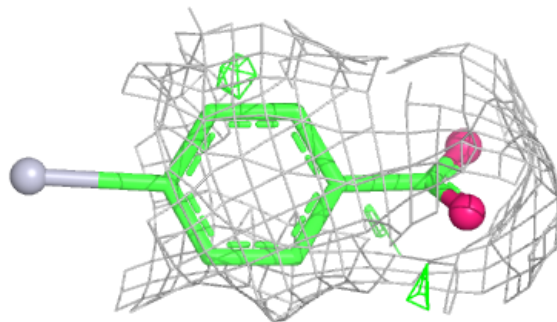
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | MBO  | D     | 301 | 10/10 | 1.00 | 0.06 | 61,75,86,93                 | 0     |
| 2   | MBO  | E     | 301 | 10/10 | 1.00 | 0.05 | 50,58,66,68                 | 0     |
| 2   | MBO  | S     | 301 | 10/10 | 1.00 | 0.05 | 74,84,89,93                 | 0     |
| 2   | MBO  | F     | 302 | 10/10 | 1.00 | 0.07 | 45,70,86,92                 | 0     |
| 3   | HG   | D     | 302 | 1/1   | 1.00 | 0.03 | 73,73,73,73                 | 0     |
| 2   | MBO  | G     | 301 | 10/10 | 1.00 | 0.06 | 52,75,79,82                 | 0     |
| 3   | HG   | F     | 301 | 1/1   | 1.00 | 0.03 | 60,60,60,60                 | 0     |
| 2   | MBO  | H     | 301 | 10/10 | 1.00 | 0.06 | 62,76,90,90                 | 0     |
| 2   | MBO  | A     | 302 | 10/10 | 1.00 | 0.07 | 68,80,85,87                 | 0     |
| 2   | MBO  | I     | 302 | 10/10 | 1.00 | 0.06 | 56,67,80,81                 | 0     |
| 2   | MBO  | B     | 301 | 10/10 | 1.00 | 0.07 | 79,97,103,105               | 0     |
| 2   | MBO  | K     | 302 | 10/10 | 1.00 | 0.07 | 72,82,90,93                 | 0     |
| 2   | MBO  | L     | 301 | 10/10 | 1.00 | 0.05 | 54,71,77,79                 | 0     |
| 2   | MBO  | L     | 302 | 10/10 | 1.00 | 0.06 | 65,86,96,100                | 0     |
| 2   | MBO  | M     | 301 | 10/10 | 1.00 | 0.07 | 63,81,100,100               | 0     |
| 2   | MBO  | B     | 302 | 10/10 | 1.00 | 0.07 | 76,103,112,112              | 0     |
| 2   | MBO  | A     | 301 | 10/10 | 1.00 | 0.06 | 61,73,77,79                 | 0     |

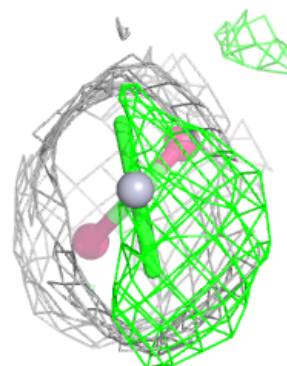
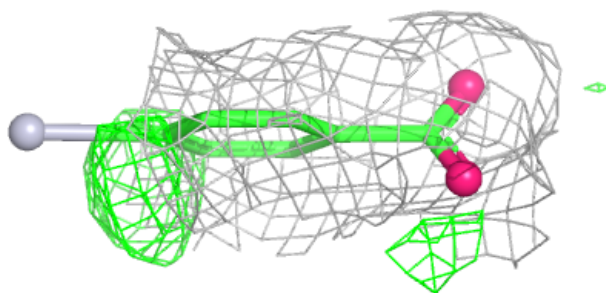
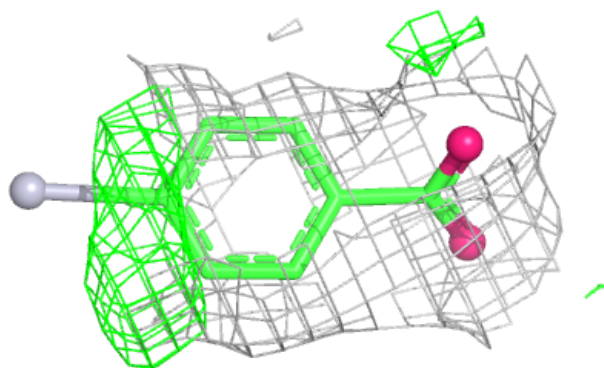
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around MBO H 302:**

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

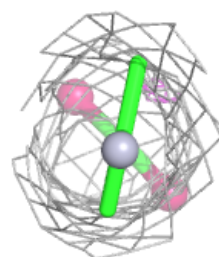
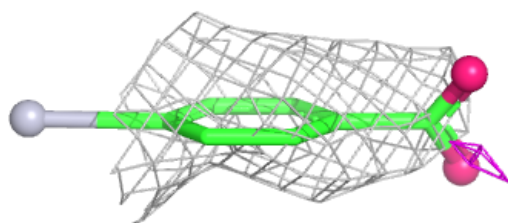
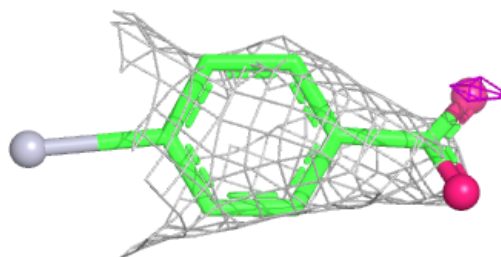
**Electron density around MBO K 301:**

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

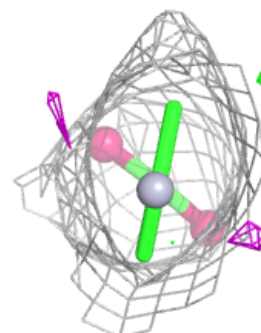
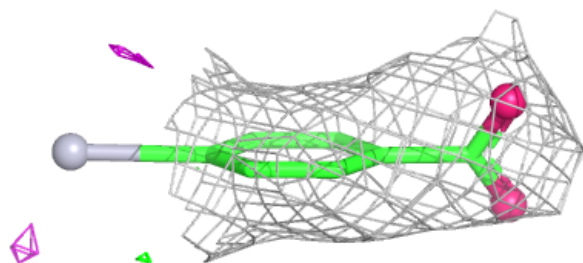
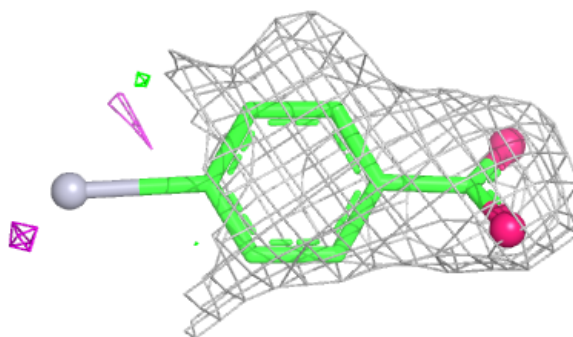


**Electron density around MBO M 302:**

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

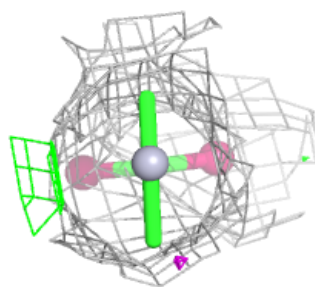
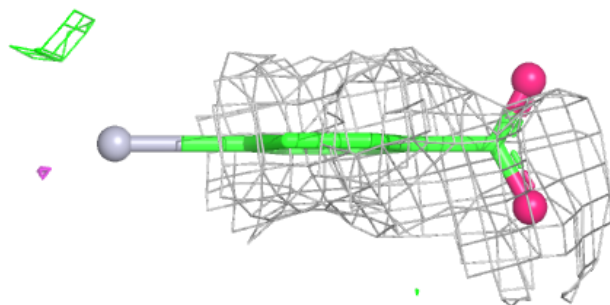
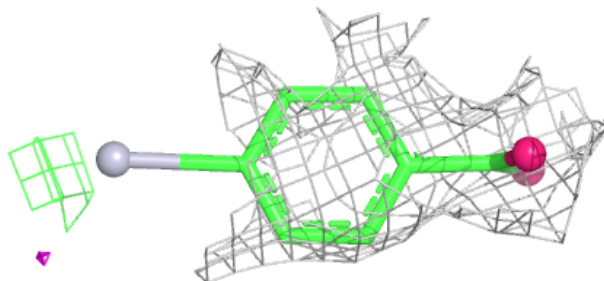
**Electron density around MBO O 301:**

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

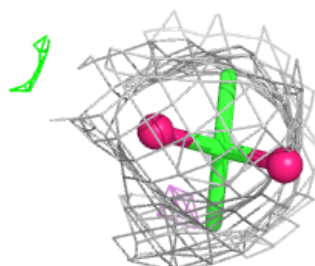
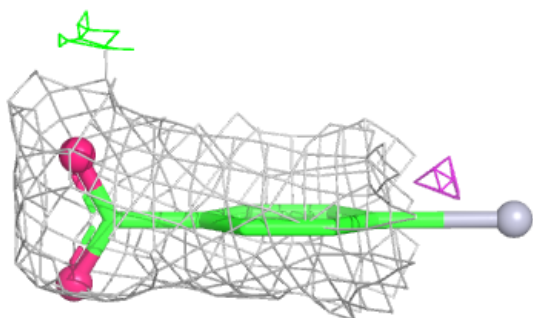
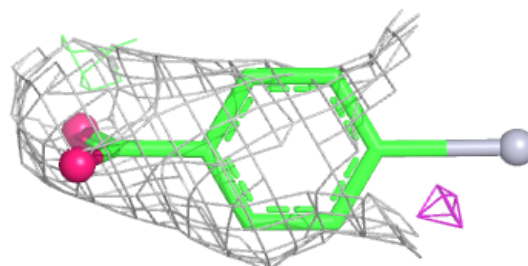


**Electron density around MBO R 301:**

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

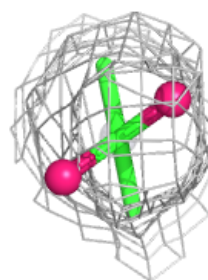
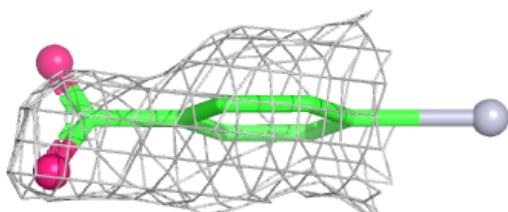
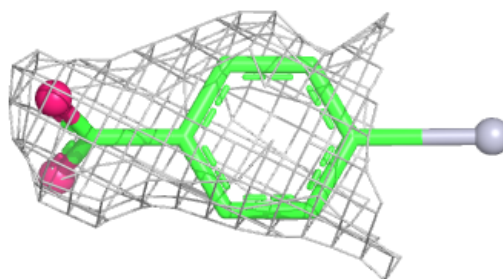
**Electron density around MBO C 301:**

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

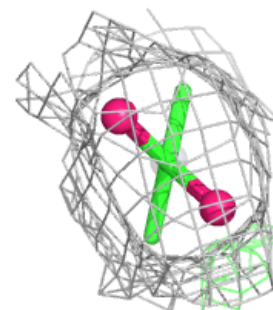
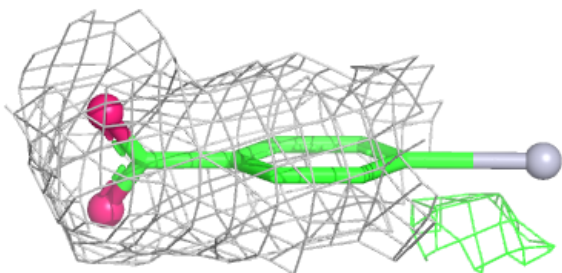
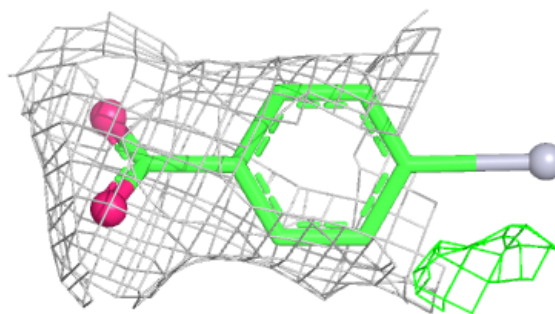


**Electron density around MBO D 301:**

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

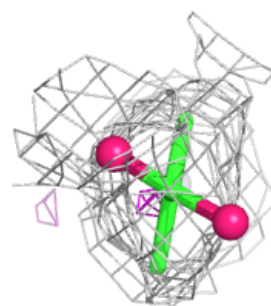
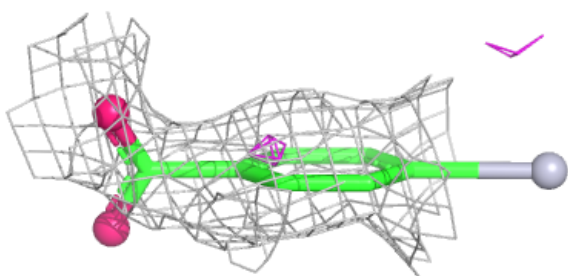
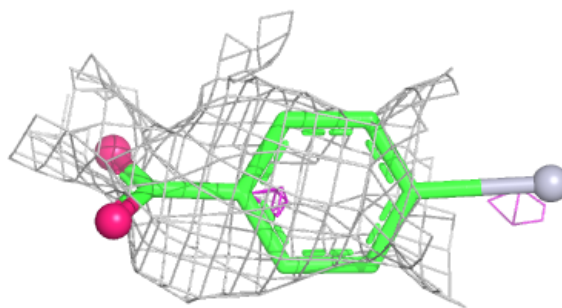
**Electron density around MBO S 301:**

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

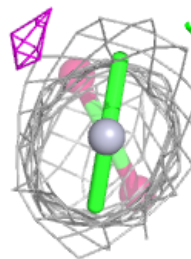
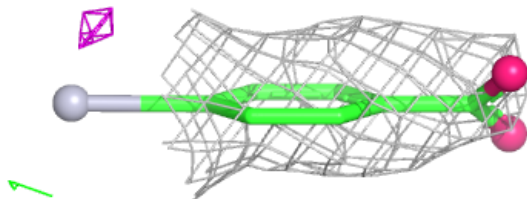
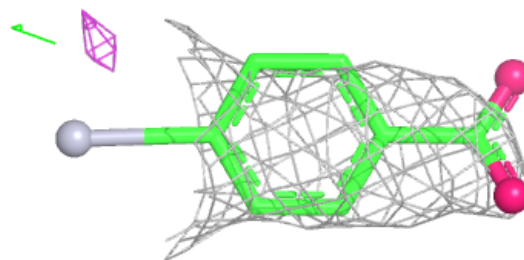


**Electron density around MBO F 302:**

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

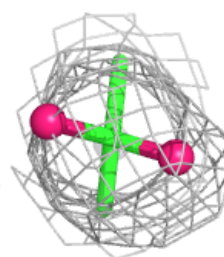
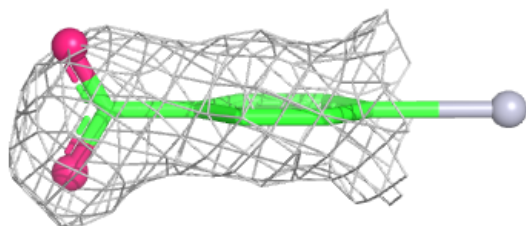
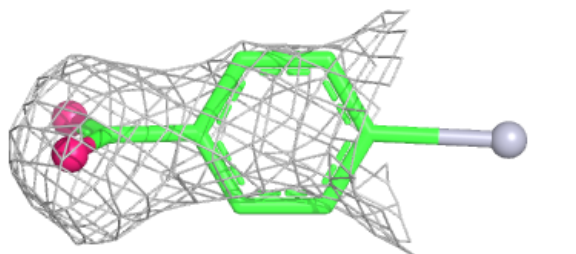
**Electron density around MBO H 301:**

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

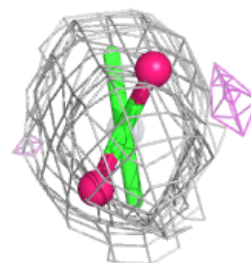
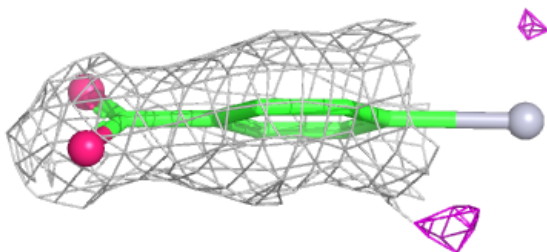
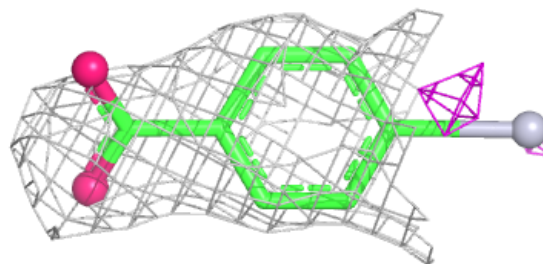


**Electron density around MBO A 302:**

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

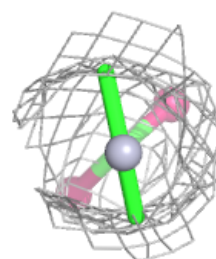
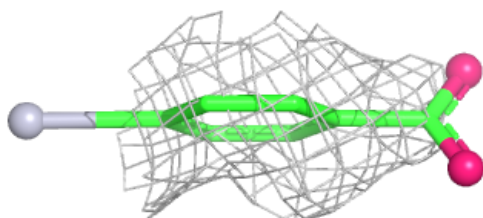
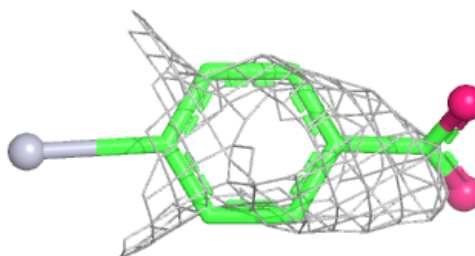
**Electron density around MBO I 302:**

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

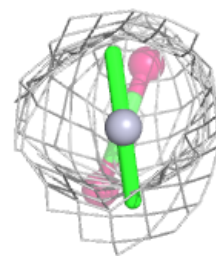
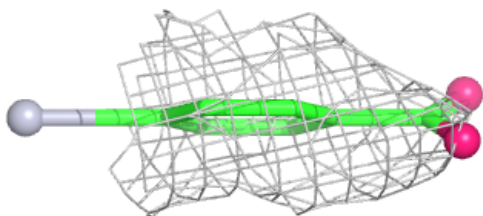
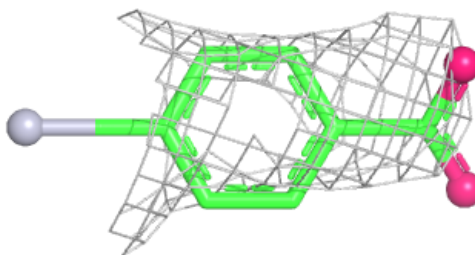


**Electron density around MBO B 301:**

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

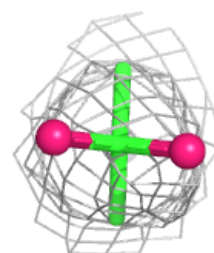
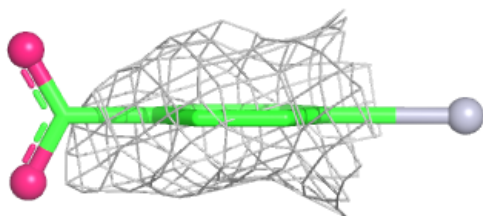
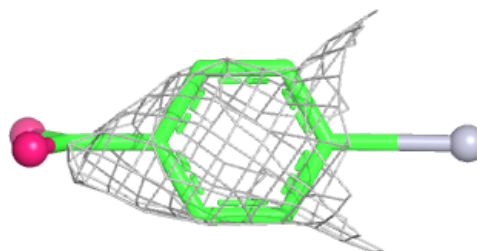
**Electron density around MBO K 302:**

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

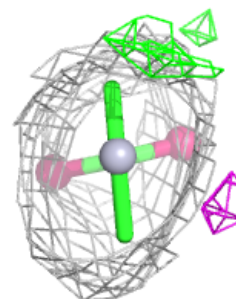
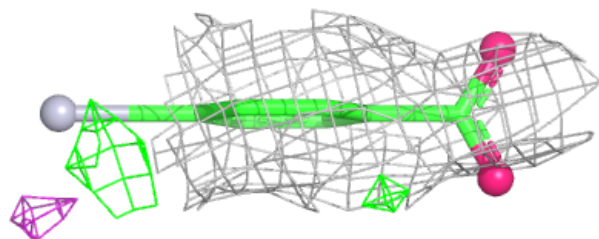
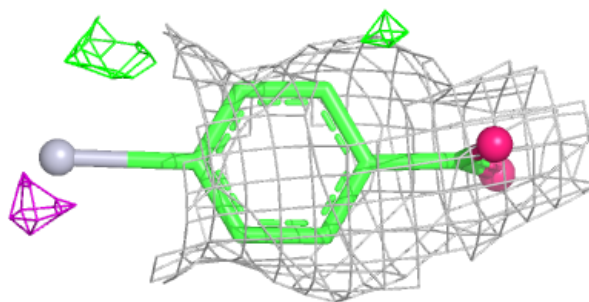


**Electron density around MBO L 302:**

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

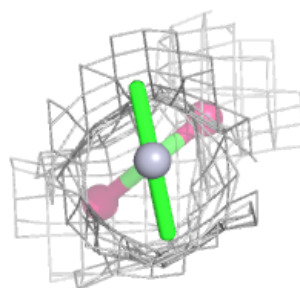
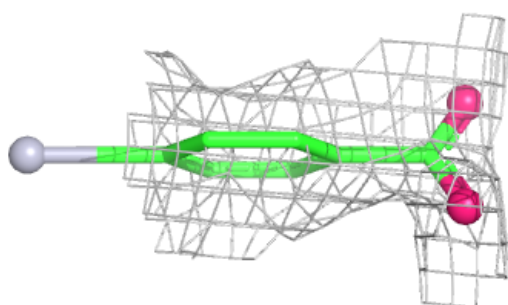
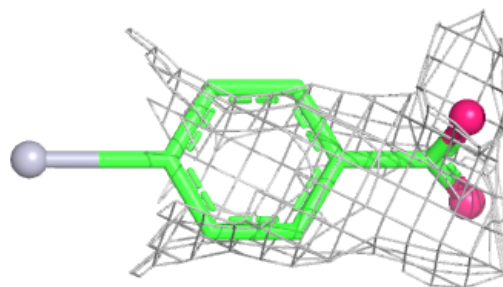
**Electron density around MBO M 301:**

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

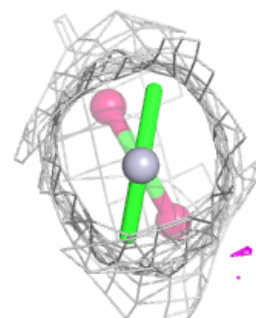
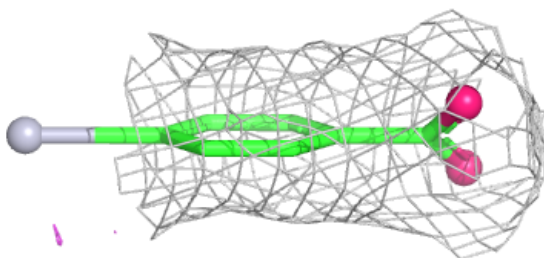
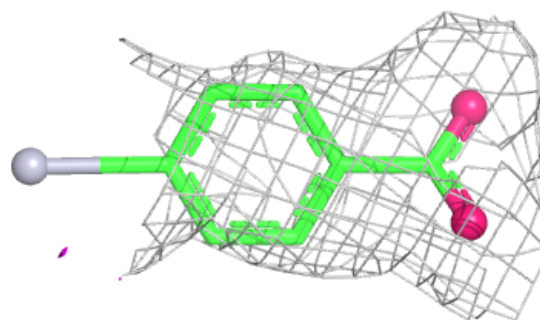


**Electron density around MBO B 302:**

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

**Electron density around MBO 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.