



# Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 10:05 AM EDT

PDB ID : 2FZS / pdb\_00002fzs  
Title : Crystal structure of E. coli ClpP with a Peptide Chloromethyl Ketone Covalently Bound at the Active Site  
Authors : Szyk, A.; Maurizi, M.R.  
Deposited on : 2006-02-10  
Resolution : 1.90 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:

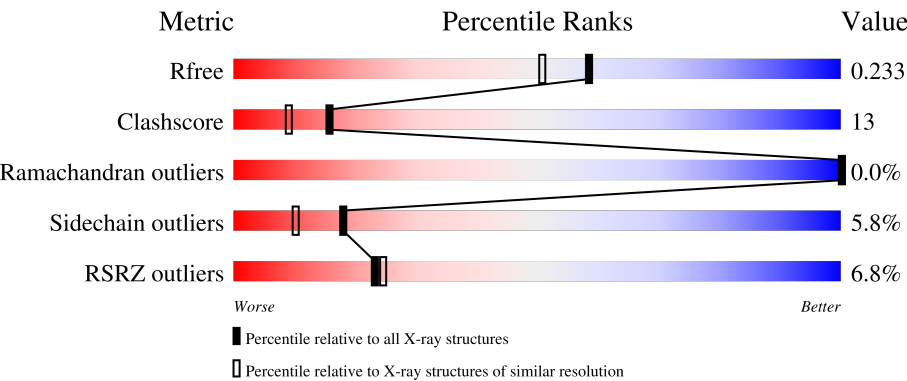
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| 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 i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 7789 (1.90-1.90)                                      |
| Clashscore            | 190562                      | 8410 (1.90-1.90)                                      |
| Ramachandran outliers | 187476                      | 8333 (1.90-1.90)                                      |
| Sidechain outliers    | 187428                      | 8333 (1.90-1.90)                                      |
| RSRZ outliers         | 180081                      | 7790 (1.90-1.90)                                      |

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     | 193    | <div><div>5%</div><div><div></div><div>74%</div><div>17%</div><div>6%</div><div></div></div><div></div></div>   |
| 1   | B     | 193    | <div><div>14%</div><div><div></div><div>77%</div><div>19%</div><div></div></div><div></div></div>               |
| 1   | C     | 193    | <div><div>7%</div><div><div></div><div>76%</div><div>13%</div><div>5%</div><div>5%</div></div><div></div></div> |
| 1   | D     | 193    | <div><div>8%</div><div><div></div><div>74%</div><div>18%</div><div></div></div><div></div></div>                |
| 1   | E     | 193    | <div><div>12%</div><div><div></div><div>76%</div><div>20%</div><div></div></div><div></div></div>               |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 193    |                  |
| 1   | G     | 193    |                  |
| 1   | H     | 193    |                  |
| 1   | I     | 193    |                  |
| 1   | J     | 193    |                  |
| 1   | K     | 193    |                  |
| 1   | L     | 193    |                  |
| 1   | M     | 193    |                  |
| 1   | N     | 193    |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 4   | GOL  | C     | 3006 | -         | -        | X       | -                |

## 2 Entry composition

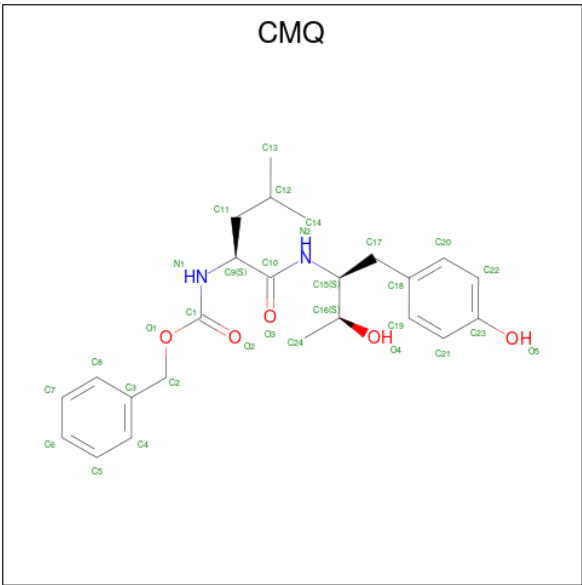
There are 5 unique types of molecules in this entry. The entry contains 24125 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-dependent Clp protease proteolytic subunit.

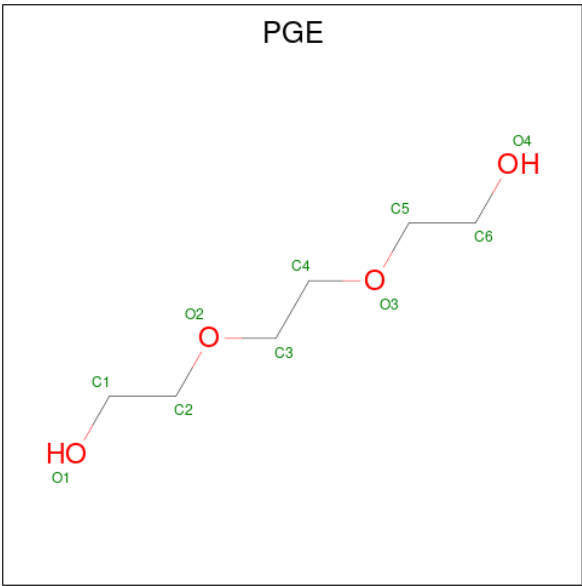
| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 1   | A     | 186      | Total | C   | N   | O   | S  | 0       | 7       | 0     |
|     |       |          | 1487  | 946 | 252 | 274 | 15 |         |         |       |
| 1   | B     | 192      | Total | C   | N   | O   | S  | 0       | 10      | 0     |
|     |       |          | 1554  | 981 | 268 | 290 | 15 |         |         |       |
| 1   | C     | 183      | Total | C   | N   | O   | S  | 0       | 7       | 0     |
|     |       |          | 1467  | 931 | 254 | 270 | 12 |         |         |       |
| 1   | D     | 185      | Total | C   | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 1462  | 926 | 249 | 275 | 12 |         |         |       |
| 1   | E     | 188      | Total | C   | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 1479  | 936 | 252 | 278 | 13 |         |         |       |
| 1   | F     | 185      | Total | C   | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 1453  | 920 | 247 | 274 | 12 |         |         |       |
| 1   | G     | 183      | Total | C   | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 1448  | 917 | 246 | 271 | 14 |         |         |       |
| 1   | H     | 183      | Total | C   | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 1439  | 912 | 245 | 270 | 12 |         |         |       |
| 1   | I     | 183      | Total | C   | N   | O   | S  | 0       | 7       | 0     |
|     |       |          | 1461  | 928 | 248 | 270 | 15 |         |         |       |
| 1   | J     | 185      | Total | C   | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 1456  | 922 | 247 | 274 | 13 |         |         |       |
| 1   | K     | 186      | Total | C   | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 1462  | 926 | 251 | 273 | 12 |         |         |       |
| 1   | L     | 183      | Total | C   | N   | O   | S  | 0       | 11      | 0     |
|     |       |          | 1478  | 939 | 246 | 278 | 15 |         |         |       |
| 1   | M     | 186      | Total | C   | N   | O   | S  | 0       | 11      | 0     |
|     |       |          | 1505  | 958 | 256 | 276 | 15 |         |         |       |
| 1   | N     | 183      | Total | C   | N   | O   | S  | 0       | 10      | 0     |
|     |       |          | 1469  | 938 | 245 | 271 | 15 |         |         |       |

- Molecule 2 is N 2 -[(BENZYLOXY)CARBONYL]-N-[(1S,2S)-2-HYDROXY-1-(4-HYDROXYBENZYL)PROPYL]-L-LEUCINAMIDE (CCD ID: CMQ) (formula: C<sub>24</sub>H<sub>32</sub>N<sub>2</sub>O<sub>5</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 31    | 24 | 2 | 5 |         |         |
| 2   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 31    | 24 | 2 | 5 |         |         |
| 2   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 31    | 24 | 2 | 5 |         |         |
| 2   | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 31    | 24 | 2 | 5 |         |         |
| 2   | E     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 31    | 24 | 2 | 5 |         |         |
| 2   | F     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 31    | 24 | 2 | 5 |         |         |
| 2   | G     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 31    | 24 | 2 | 5 |         |         |
| 2   | H     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 31    | 24 | 2 | 5 |         |         |
| 2   | I     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 31    | 24 | 2 | 5 |         |         |
| 2   | J     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 31    | 24 | 2 | 5 |         |         |
| 2   | K     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 31    | 24 | 2 | 5 |         |         |
| 2   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 31    | 24 | 2 | 5 |         |         |
| 2   | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 31    | 24 | 2 | 5 |         |         |
| 2   | N     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 31    | 24 | 2 | 5 |         |         |

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 3   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 3   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 3   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 3   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 3   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 3   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 3   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 3   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 3   | J     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 3   | K     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 3   | K     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 3   | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | M     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 3   | N     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 4   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 4   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 4   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 4   | K     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 4   | N     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

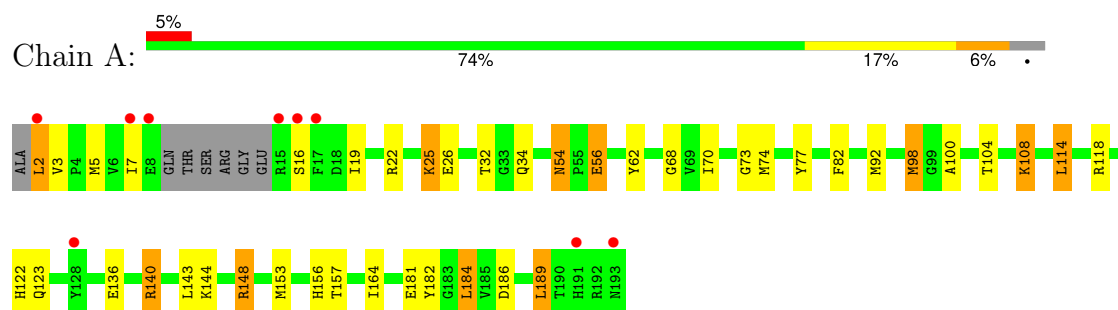
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 5   | A     | 234      | Total | O   | 0       | 0       |
|     |       |          | 234   | 234 |         |         |
| 5   | B     | 188      | Total | O   | 0       | 0       |
|     |       |          | 188   | 188 |         |         |
| 5   | C     | 189      | Total | O   | 0       | 0       |
|     |       |          | 189   | 189 |         |         |
| 5   | D     | 165      | Total | O   | 0       | 0       |
|     |       |          | 165   | 165 |         |         |
| 5   | E     | 199      | Total | O   | 0       | 0       |
|     |       |          | 199   | 199 |         |         |
| 5   | F     | 218      | Total | O   | 0       | 0       |
|     |       |          | 218   | 218 |         |         |
| 5   | G     | 232      | Total | O   | 0       | 0       |
|     |       |          | 232   | 232 |         |         |
| 5   | H     | 176      | Total | O   | 0       | 0       |
|     |       |          | 176   | 176 |         |         |
| 5   | I     | 171      | Total | O   | 0       | 0       |
|     |       |          | 171   | 171 |         |         |
| 5   | J     | 176      | Total | O   | 0       | 0       |
|     |       |          | 176   | 176 |         |         |
| 5   | K     | 192      | Total | O   | 0       | 0       |
|     |       |          | 192   | 192 |         |         |
| 5   | L     | 247      | Total | O   | 0       | 0       |
|     |       |          | 247   | 247 |         |         |
| 5   | M     | 251      | Total | O   | 0       | 0       |
|     |       |          | 251   | 251 |         |         |
| 5   | N     | 217      | Total | O   | 0       | 0       |
|     |       |          | 217   | 217 |         |         |

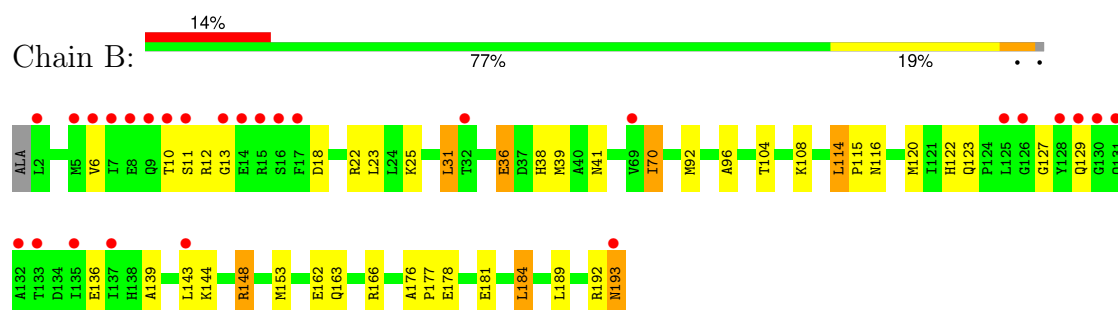
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

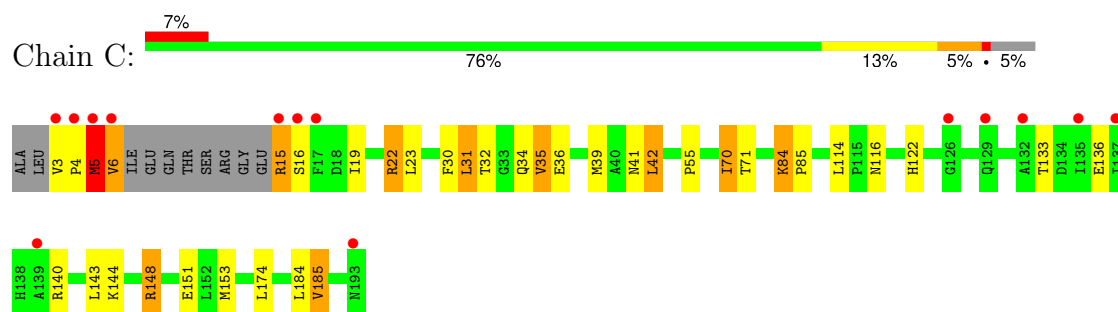
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

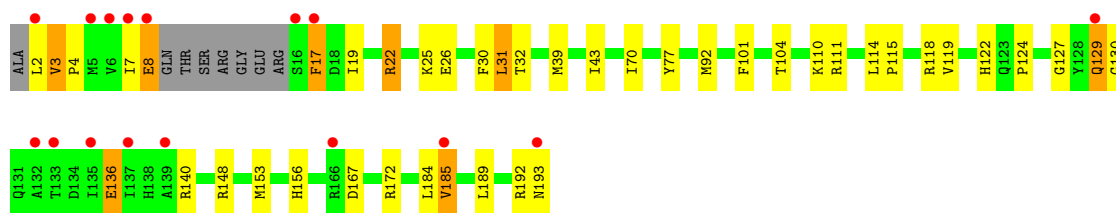


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

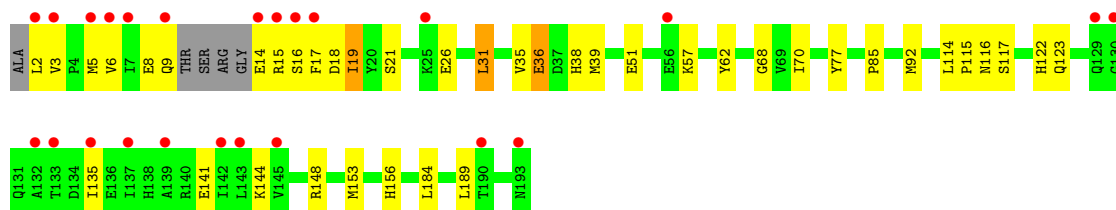
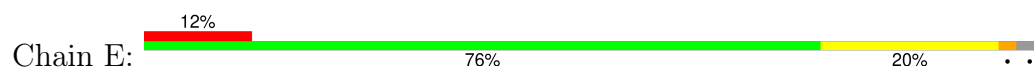


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

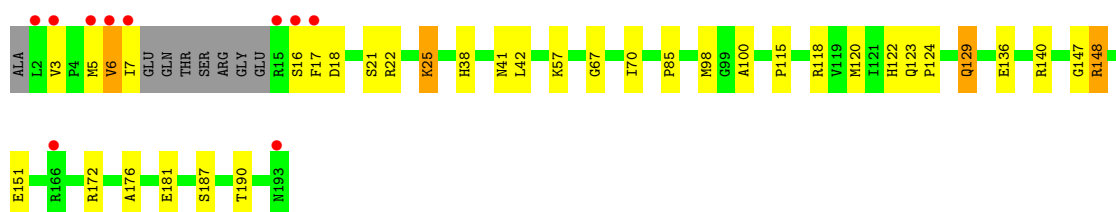
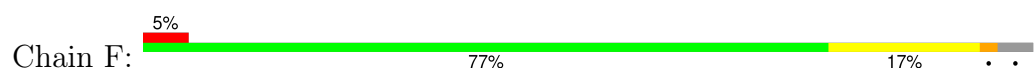




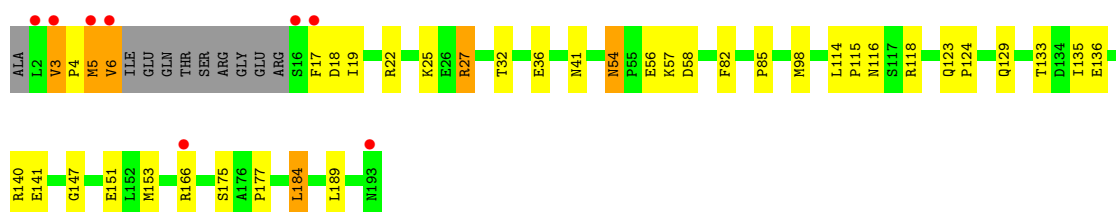
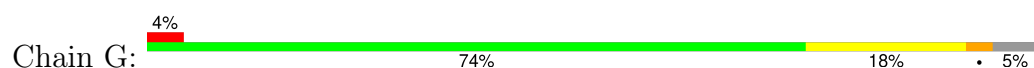
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



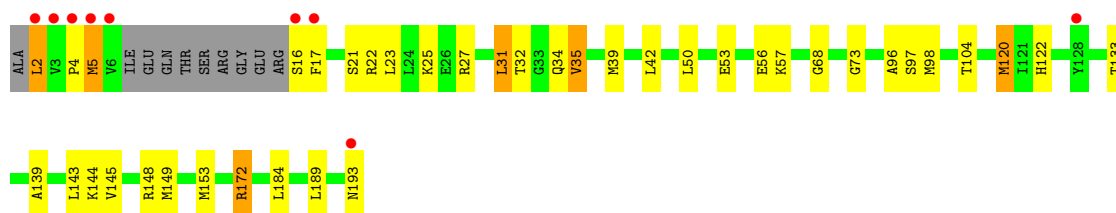
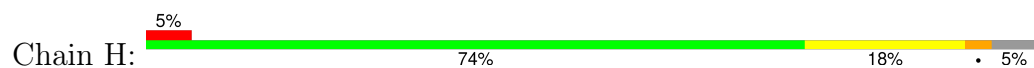
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



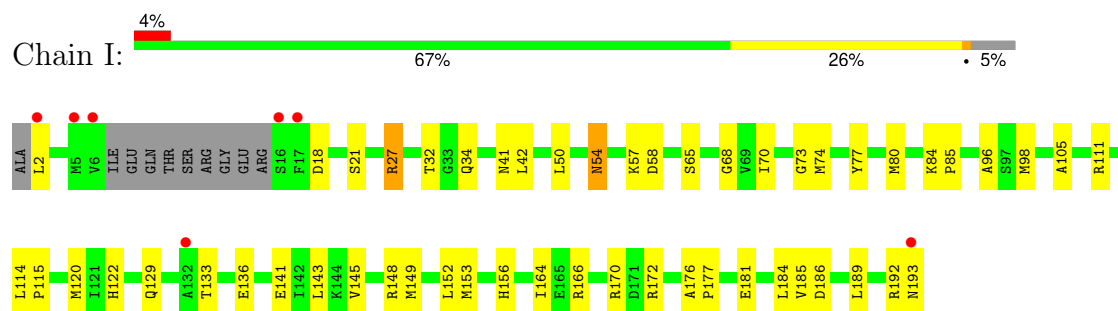
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



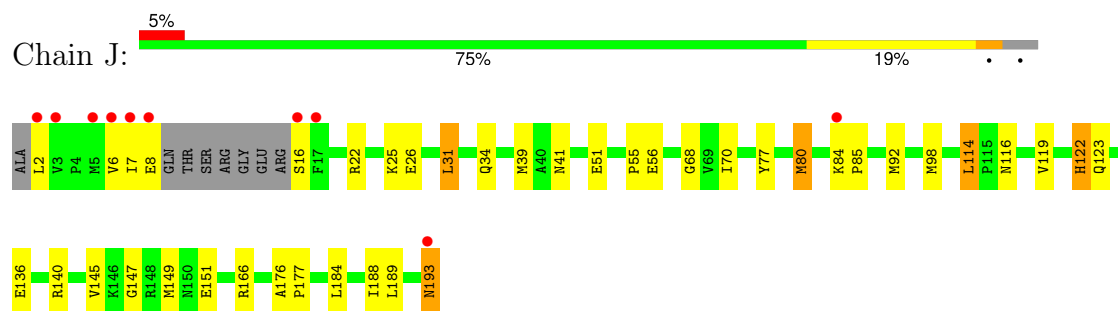
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



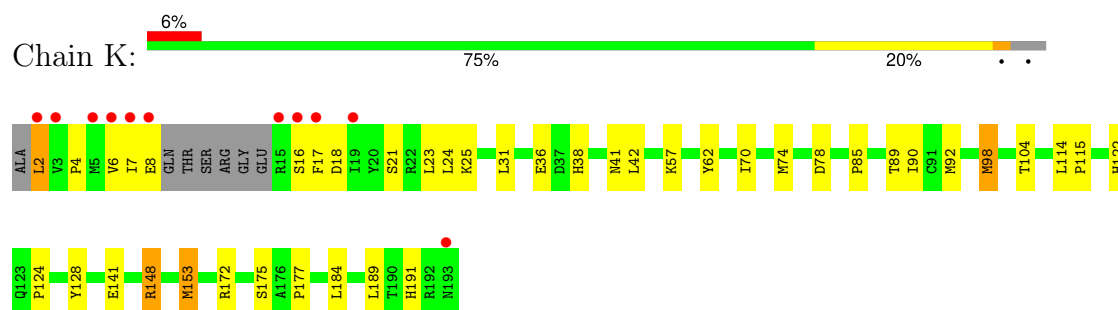
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



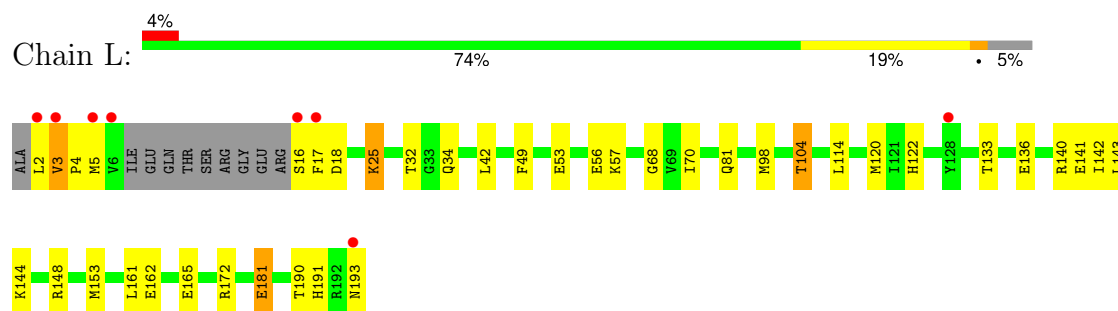
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



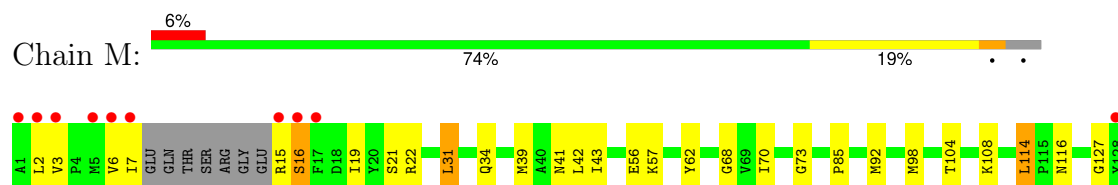
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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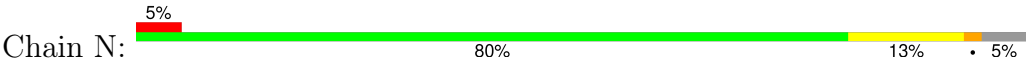


- Molecule 1: ATP-dependent Clp protease proteolytic subunit





● Molecule 1: ATP-dependent Clp protease proteolytic subunit



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 190.70Å 101.00Å 155.40Å<br>90.00° 99.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 15.00 – 1.90<br>15.00 – 1.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 93.8 (15.00-1.90)<br>93.6 (15.00-1.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.05                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.16 (at 1.89Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0005                                             | Depositor        |
| R, $R_{free}$                                                           | 0.173 , 0.233<br>0.174 , 0.233                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 10777 reflections (4.68%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 27.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.223                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 41.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 24125                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 35.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: PGE, CMQ, GOL

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     | 1.09         | 2/1538 (0.1%)   | 1.02        | 0/2069          |
| 1   | B     | 0.99         | 0/1618          | 1.04        | 2/2175 (0.1%)   |
| 1   | C     | 1.01         | 0/1518          | 1.09        | 4/2043 (0.2%)   |
| 1   | D     | 0.98         | 3/1497 (0.2%)   | 1.04        | 1/2016 (0.0%)   |
| 1   | E     | 1.09         | 0/1510          | 1.03        | 1/2032 (0.0%)   |
| 1   | F     | 1.28         | 3/1484 (0.2%)   | 1.15        | 4/1999 (0.2%)   |
| 1   | G     | 1.21         | 2/1487 (0.1%)   | 1.22        | 7/2001 (0.3%)   |
| 1   | H     | 1.01         | 0/1470          | 1.06        | 2/1980 (0.1%)   |
| 1   | I     | 0.91         | 0/1512          | 1.04        | 5/2034 (0.2%)   |
| 1   | J     | 0.92         | 0/1487          | 1.02        | 0/2002          |
| 1   | K     | 1.03         | 0/1489          | 1.06        | 1/2006 (0.0%)   |
| 1   | L     | 1.13         | 0/1545          | 1.02        | 0/2079          |
| 1   | M     | 1.17         | 1/1572 (0.1%)   | 1.08        | 1/2113 (0.0%)   |
| 1   | N     | 1.06         | 2/1532 (0.1%)   | 1.02        | 2/2063 (0.1%)   |
| All | All   | 1.07         | 13/21259 (0.1%) | 1.06        | 30/28612 (0.1%) |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | F     | 176 | ALA  | CA-CB | 7.75  | 1.63        | 1.53     |
| 1   | G     | 27  | ARG  | CD-NE | -6.74 | 1.36        | 1.46     |
| 1   | D     | 19  | ILE  | CA-CB | 5.88  | 1.60        | 1.54     |
| 1   | F     | 67  | GLY  | C-O   | -5.63 | 1.20        | 1.24     |
| 1   | A     | 100 | ALA  | C-O   | 5.60  | 1.30        | 1.24     |
| 1   | D     | 111 | ARG  | N-CA  | 5.57  | 1.52        | 1.46     |
| 1   | N     | 126 | GLY  | C-O   | -5.46 | 1.18        | 1.23     |
| 1   | M     | 176 | ALA  | CA-C  | 5.30  | 1.59        | 1.52     |
| 1   | D     | 110 | LYS  | CA-C  | 5.20  | 1.59        | 1.52     |
| 1   | A     | 164 | ILE  | N-CA  | 5.17  | 1.52        | 1.46     |
| 1   | N     | 164 | ILE  | CA-CB | 5.13  | 1.60        | 1.54     |
| 1   | G     | 98  | MET  | N-CA  | 5.08  | 1.52        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | F     | 100 | ALA  | N-CA  | 5.04 | 1.52        | 1.46     |

All (30) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | G     | 27  | ARG  | NE-CZ-NH2 | -14.72 | 105.95      | 119.20   |
| 1   | G     | 27  | ARG  | CD-NE-CZ  | 9.54   | 137.75      | 124.40   |
| 1   | G     | 27  | ARG  | NE-CZ-NH1 | 8.83   | 130.33      | 121.50   |
| 1   | G     | 27  | ARG  | CG-CD-NE  | -8.38  | 93.56       | 112.00   |
| 1   | G     | 3   | VAL  | CA-C-N    | 8.22   | 128.73      | 119.93   |
| 1   | G     | 3   | VAL  | C-N-CA    | 8.22   | 128.73      | 119.93   |
| 1   | K     | 98  | MET  | CG-SD-CE  | -7.45  | 84.52       | 100.90   |
| 1   | M     | 16  | SER  | N-CA-C    | 7.02   | 119.63      | 110.43   |
| 1   | N     | 118 | ARG  | CG-CD-NE  | -6.82  | 97.00       | 112.00   |
| 1   | C     | 35  | VAL  | N-CA-CB   | 6.73   | 117.86      | 110.53   |
| 1   | D     | 185 | VAL  | CB-CA-C   | 6.69   | 122.68      | 110.71   |
| 1   | I     | 54  | ASN  | CA-C-N    | 6.32   | 127.74      | 119.84   |
| 1   | I     | 54  | ASN  | C-N-CA    | 6.32   | 127.74      | 119.84   |
| 1   | G     | 5   | MET  | N-CA-C    | 6.07   | 118.83      | 108.02   |
| 1   | I     | 156 | HIS  | N-CA-C    | 5.95   | 119.01      | 111.69   |
| 1   | H     | 35  | VAL  | CB-CA-C   | 5.94   | 118.87      | 111.15   |
| 1   | F     | 98  | MET  | CG-SD-CE  | -5.71  | 88.33       | 100.90   |
| 1   | E     | 68  | GLY  | N-CA-C    | 5.45   | 117.36      | 110.38   |
| 1   | F     | 70  | ILE  | N-CA-C    | 5.44   | 115.64      | 110.42   |
| 1   | B     | 36  | GLU  | CA-CB-CG  | 5.37   | 124.84      | 114.10   |
| 1   | C     | 185 | VAL  | CB-CA-C   | 5.34   | 119.33      | 110.30   |
| 1   | F     | 124 | PRO  | CB-CA-C   | -5.24  | 104.52      | 111.23   |
| 1   | N     | 59  | ILE  | N-CA-C    | -5.24  | 100.94      | 108.48   |
| 1   | I     | 65  | SER  | CA-C-N    | 5.18   | 125.64      | 120.04   |
| 1   | I     | 65  | SER  | C-N-CA    | 5.18   | 125.64      | 120.04   |
| 1   | C     | 70  | ILE  | N-CA-C    | 5.17   | 115.39      | 110.42   |
| 1   | F     | 120 | MET  | CG-SD-CE  | -5.15  | 89.56       | 100.90   |
| 1   | C     | 5   | MET  | N-CA-C    | 5.11   | 116.64      | 108.41   |
| 1   | B     | 70  | ILE  | N-CA-C    | 5.10   | 115.32      | 110.42   |
| 1   | H     | 53  | GLU  | N-CA-C    | 5.05   | 116.78      | 111.28   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1487  | 0        | 1509     | 65      | 0            |
| 1   | B     | 1554  | 0        | 1567     | 57      | 0            |
| 1   | C     | 1467  | 0        | 1487     | 45      | 0            |
| 1   | D     | 1462  | 0        | 1471     | 51      | 0            |
| 1   | E     | 1479  | 0        | 1486     | 43      | 0            |
| 1   | F     | 1453  | 0        | 1456     | 21      | 0            |
| 1   | G     | 1448  | 0        | 1455     | 40      | 0            |
| 1   | H     | 1439  | 0        | 1448     | 43      | 0            |
| 1   | I     | 1461  | 0        | 1477     | 51      | 0            |
| 1   | J     | 1456  | 0        | 1463     | 39      | 0            |
| 1   | K     | 1462  | 0        | 1476     | 47      | 0            |
| 1   | L     | 1478  | 0        | 1483     | 47      | 0            |
| 1   | M     | 1505  | 0        | 1533     | 44      | 0            |
| 1   | N     | 1469  | 0        | 1492     | 26      | 0            |
| 2   | A     | 31    | 0        | 31       | 9       | 0            |
| 2   | B     | 31    | 0        | 30       | 7       | 0            |
| 2   | C     | 31    | 0        | 30       | 6       | 0            |
| 2   | D     | 31    | 0        | 31       | 8       | 0            |
| 2   | E     | 31    | 0        | 31       | 8       | 0            |
| 2   | F     | 31    | 0        | 28       | 1       | 0            |
| 2   | G     | 31    | 0        | 29       | 1       | 0            |
| 2   | H     | 31    | 0        | 31       | 6       | 0            |
| 2   | I     | 31    | 0        | 31       | 7       | 0            |
| 2   | J     | 31    | 0        | 31       | 8       | 0            |
| 2   | K     | 31    | 0        | 31       | 9       | 0            |
| 2   | L     | 31    | 0        | 29       | 7       | 0            |
| 2   | M     | 31    | 0        | 29       | 1       | 0            |
| 2   | N     | 31    | 0        | 29       | 2       | 0            |
| 3   | A     | 10    | 0        | 14       | 1       | 0            |
| 3   | B     | 10    | 0        | 14       | 2       | 0            |
| 3   | C     | 10    | 0        | 14       | 0       | 0            |
| 3   | D     | 10    | 0        | 14       | 0       | 0            |
| 3   | E     | 10    | 0        | 14       | 0       | 0            |
| 3   | F     | 10    | 0        | 14       | 1       | 0            |
| 3   | G     | 10    | 0        | 14       | 0       | 0            |
| 3   | H     | 10    | 0        | 14       | 0       | 0            |
| 3   | I     | 10    | 0        | 14       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | J     | 10    | 0        | 14       | 1       | 0            |
| 3   | K     | 20    | 0        | 28       | 2       | 0            |
| 3   | L     | 10    | 0        | 14       | 0       | 0            |
| 3   | M     | 10    | 0        | 14       | 1       | 0            |
| 3   | N     | 10    | 0        | 14       | 2       | 0            |
| 4   | A     | 6     | 0        | 8        | 2       | 0            |
| 4   | B     | 12    | 0        | 16       | 0       | 0            |
| 4   | C     | 12    | 0        | 16       | 6       | 0            |
| 4   | F     | 6     | 0        | 8        | 2       | 0            |
| 4   | G     | 6     | 0        | 8        | 1       | 0            |
| 4   | H     | 6     | 0        | 8        | 2       | 0            |
| 4   | K     | 6     | 0        | 8        | 1       | 0            |
| 4   | L     | 6     | 0        | 8        | 0       | 0            |
| 4   | N     | 6     | 0        | 8        | 3       | 0            |
| 5   | A     | 234   | 0        | 0        | 13      | 0            |
| 5   | B     | 188   | 0        | 0        | 6       | 0            |
| 5   | C     | 189   | 0        | 0        | 8       | 0            |
| 5   | D     | 165   | 0        | 0        | 5       | 0            |
| 5   | E     | 199   | 0        | 0        | 10      | 0            |
| 5   | F     | 218   | 0        | 0        | 7       | 0            |
| 5   | G     | 232   | 0        | 0        | 8       | 0            |
| 5   | H     | 176   | 0        | 0        | 5       | 0            |
| 5   | I     | 171   | 0        | 0        | 5       | 0            |
| 5   | J     | 176   | 0        | 0        | 6       | 0            |
| 5   | K     | 192   | 0        | 0        | 8       | 0            |
| 5   | L     | 247   | 0        | 0        | 12      | 0            |
| 5   | M     | 251   | 0        | 0        | 5       | 0            |
| 5   | N     | 217   | 0        | 0        | 6       | 0            |
| All | All   | 24125 | 0        | 21522    | 563     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (563) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:122:HIS:NE2 | 2:D:504:CMQ:H242 | 1.14                     | 1.45              |
| 1:I:122:HIS:NE2 | 2:I:509:CMQ:H242 | 1.24                     | 1.45              |
| 1:B:122:HIS:NE2 | 2:B:502:CMQ:H242 | 1.20                     | 1.43              |
| 1:H:122:HIS:NE2 | 2:H:508:CMQ:H242 | 1.14                     | 1.43              |
| 1:A:122:HIS:NE2 | 2:A:501:CMQ:H242 | 1.20                     | 1.41              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:C:122:HIS:NE2    | 2:C:503:CMQ:H242    | 1.31                     | 1.41              |
| 1:J:122:HIS:NE2    | 2:J:510:CMQ:H242    | 1.09                     | 1.41              |
| 1:E:122:HIS:NE2    | 2:E:505:CMQ:H242    | 1.11                     | 1.40              |
| 1:K:122:HIS:NE2    | 2:K:511:CMQ:H242    | 1.08                     | 1.36              |
| 1:A:181:GLU:HG2    | 5:A:4202:HOH:O      | 1.40                     | 1.19              |
| 1:A:182:TYR:HD2    | 1:A:184[B]:LEU:CD2  | 1.62                     | 1.12              |
| 1:K:104:THR:HG21   | 1:K:153:MET:HE1     | 1.23                     | 1.10              |
| 1:C:6:VAL:HG11     | 1:C:22:ARG:HH22     | 1.14                     | 1.07              |
| 4:C:3006:GOL:H31   | 5:D:4147:HOH:O      | 1.54                     | 1.06              |
| 1:C:15:ARG:HG2     | 1:C:15:ARG:HH11     | 0.94                     | 1.04              |
| 1:I:77:TYR:HA      | 1:I:80:MET:HE2      | 1.35                     | 1.04              |
| 1:H:122:HIS:NE2    | 2:H:508:CMQ:H241    | 1.72                     | 1.03              |
| 1:K:104:THR:HG21   | 1:K:153:MET:CE      | 1.89                     | 1.01              |
| 1:K:104:THR:CG2    | 1:K:153:MET:HE1     | 1.90                     | 1.01              |
| 1:L:136[B]:GLU:OE2 | 1:L:140:ARG:HD3     | 1.60                     | 1.00              |
| 1:A:182:TYR:HD2    | 1:A:184[B]:LEU:HD21 | 1.25                     | 0.99              |
| 1:F:22:ARG:O       | 1:F:25:LYS:HG2      | 1.62                     | 0.99              |
| 1:A:182:TYR:CD2    | 1:A:184[B]:LEU:HD21 | 1.99                     | 0.96              |
| 1:H:122:HIS:CD2    | 2:H:508:CMQ:H242    | 2.02                     | 0.93              |
| 1:C:22:ARG:HH11    | 1:C:22:ARG:HB2      | 1.30                     | 0.93              |
| 1:I:122:HIS:NE2    | 2:I:509:CMQ:H241    | 1.79                     | 0.93              |
| 1:L:98[B]:MET:HE2  | 2:L:512:CMQ:C17     | 1.99                     | 0.93              |
| 1:E:153:MET:HE3    | 5:E:4193:HOH:O      | 1.66                     | 0.93              |
| 1:B:122:HIS:NE2    | 2:B:502:CMQ:H241    | 1.83                     | 0.92              |
| 1:J:77:TYR:HA      | 1:J:80[A]:MET:HE2   | 1.51                     | 0.92              |
| 2:G:507:CMQ:H7     | 5:G:4221:HOH:O      | 1.68                     | 0.92              |
| 1:A:182:TYR:CD2    | 1:A:184[B]:LEU:CD2  | 2.53                     | 0.92              |
| 1:C:15:ARG:HG2     | 1:C:15:ARG:NH1      | 1.73                     | 0.91              |
| 1:B:148[A]:ARG:NH1 | 1:C:116:ASN:HD21    | 1.70                     | 0.89              |
| 1:F:172:ARG:HD3    | 5:F:4165:HOH:O      | 1.71                     | 0.89              |
| 1:G:3:VAL:CG1      | 1:G:18:ASP:HB2      | 2.03                     | 0.88              |
| 1:L:98[B]:MET:HE2  | 2:L:512:CMQ:H172    | 1.55                     | 0.88              |
| 1:F:136[B]:GLU:HG3 | 1:M:143:LEU:HD11    | 1.53                     | 0.88              |
| 1:K:122:HIS:NE2    | 2:K:511:CMQ:H241    | 1.86                     | 0.88              |
| 1:C:15:ARG:HH11    | 1:C:15:ARG:CG       | 1.86                     | 0.87              |
| 1:A:92:MET:SD      | 5:A:4166:HOH:O      | 2.32                     | 0.87              |
| 2:F:506:CMQ:H7     | 5:F:4167:HOH:O      | 1.73                     | 0.86              |
| 1:A:122:HIS:CE1    | 2:A:501:CMQ:C24     | 2.56                     | 0.86              |
| 1:G:184:LEU:HB3    | 5:G:4137:HOH:O      | 1.75                     | 0.86              |
| 5:D:4094:HOH:O     | 1:E:92:MET:SD       | 2.33                     | 0.86              |
| 1:A:122:HIS:NE2    | 2:A:501:CMQ:H241    | 1.91                     | 0.86              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:J:122:HIS:CE1     | 2:J:510:CMQ:H242    | 2.10                     | 0.86              |
| 1:A:104:THR:HG21    | 1:A:153[B]:MET:CE   | 2.06                     | 0.86              |
| 4:C:3006:GOL:O3     | 1:D:118:ARG:HB2     | 1.76                     | 0.86              |
| 1:K:122:HIS:CD2     | 2:K:511:CMQ:H242    | 2.11                     | 0.85              |
| 1:D:148:ARG:HH21    | 1:E:116:ASN:HD21    | 1.25                     | 0.85              |
| 1:L:181[B]:GLU:HG2  | 5:L:4092:HOH:O      | 1.76                     | 0.85              |
| 1:B:148[A]:ARG:HH11 | 1:C:116:ASN:ND2     | 1.74                     | 0.85              |
| 1:K:122:HIS:CE1     | 2:K:511:CMQ:C24     | 2.59                     | 0.85              |
| 1:G:184:LEU:HD22    | 5:G:4137:HOH:O      | 1.74                     | 0.85              |
| 1:A:104:THR:HG21    | 1:A:153[B]:MET:HE2  | 1.56                     | 0.84              |
| 1:E:153:MET:CE      | 5:E:4193:HOH:O      | 2.23                     | 0.84              |
| 1:C:6:VAL:HG11      | 1:C:22:ARG:NH2      | 1.91                     | 0.84              |
| 1:H:172:ARG:HH11    | 1:H:172:ARG:CG      | 1.91                     | 0.83              |
| 1:N:142[B]:ILE:HD11 | 5:N:4145:HOH:O      | 1.77                     | 0.83              |
| 1:I:153[B]:MET:CE   | 1:I:184:LEU:HD21    | 2.08                     | 0.83              |
| 1:A:92:MET:HE1      | 5:G:4106:HOH:O      | 1.78                     | 0.82              |
| 1:I:122:HIS:CD2     | 2:I:509:CMQ:H242    | 2.13                     | 0.82              |
| 1:B:136:GLU:HG3     | 5:B:4185:HOH:O      | 1.80                     | 0.82              |
| 1:H:122:HIS:CE1     | 2:H:508:CMQ:H241    | 2.15                     | 0.81              |
| 1:K:184:LEU:HB3     | 5:K:4179:HOH:O      | 1.79                     | 0.81              |
| 1:J:119:VAL:HG11    | 1:J:184:LEU:HD13    | 1.61                     | 0.81              |
| 1:A:182:TYR:HD2     | 1:A:184[B]:LEU:HD23 | 1.41                     | 0.81              |
| 1:K:153:MET:HG3     | 5:K:4134:HOH:O      | 1.81                     | 0.81              |
| 1:A:148:ARG:HH11    | 1:B:116:ASN:HD21    | 1.30                     | 0.80              |
| 1:D:122:HIS:CE1     | 2:D:504:CMQ:C24     | 2.65                     | 0.80              |
| 1:D:122:HIS:CE1     | 2:D:504:CMQ:H242    | 2.13                     | 0.80              |
| 1:E:122:HIS:CE1     | 2:E:505:CMQ:C24     | 2.64                     | 0.80              |
| 1:M:104:THR:HB      | 1:M:184[B]:LEU:HD12 | 1.64                     | 0.80              |
| 1:I:153[B]:MET:HE1  | 1:I:184:LEU:HD21    | 1.65                     | 0.79              |
| 1:A:26:GLU:HG2      | 5:A:4235:HOH:O      | 1.82                     | 0.79              |
| 1:A:153[A]:MET:HG3  | 5:A:4117:HOH:O      | 1.80                     | 0.79              |
| 1:B:122:HIS:CE1     | 2:B:502:CMQ:C24     | 2.65                     | 0.79              |
| 1:E:122:HIS:NE2     | 2:E:505:CMQ:H241    | 1.96                     | 0.79              |
| 1:K:122:HIS:CE1     | 2:K:511:CMQ:H241    | 2.18                     | 0.79              |
| 1:B:143:LEU:HD11    | 1:I:136:GLU:HG3     | 1.65                     | 0.78              |
| 1:A:122:HIS:CE1     | 2:A:501:CMQ:H242    | 2.14                     | 0.78              |
| 1:J:122:HIS:CE1     | 2:J:510:CMQ:C24     | 2.67                     | 0.78              |
| 1:L:98[B]:MET:CE    | 2:L:512:CMQ:H172    | 2.13                     | 0.78              |
| 1:A:122:HIS:CE1     | 2:A:501:CMQ:H241    | 2.17                     | 0.78              |
| 1:H:122:HIS:CE1     | 2:H:508:CMQ:C24     | 2.65                     | 0.78              |
| 1:A:157:THR:HG22    | 1:A:184[B]:LEU:HD22 | 1.66                     | 0.78              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:F:118:ARG:HB3     | 4:F:3004:GOL:O3     | 1.83                     | 0.78              |
| 1:D:101:PHE:HA      | 1:D:153:MET:CE      | 2.14                     | 0.77              |
| 1:F:6:VAL:HG21      | 1:F:22:ARG:HD3      | 1.65                     | 0.77              |
| 1:B:148[A]:ARG:HH11 | 1:C:116:ASN:HD21    | 1.26                     | 0.77              |
| 1:K:92:MET:SD       | 5:K:4113:HOH:O      | 2.43                     | 0.76              |
| 1:B:163:GLN:HE22    | 1:B:166[B]:ARG:HH22 | 1.33                     | 0.76              |
| 1:C:122:HIS:NE2     | 2:C:503:CMQ:H241    | 1.99                     | 0.76              |
| 2:E:505:CMQ:H6      | 5:E:4152:HOH:O      | 1.86                     | 0.76              |
| 1:B:122:HIS:CE1     | 2:B:502:CMQ:H241    | 2.20                     | 0.75              |
| 1:K:2:LEU:HD12      | 5:K:4177:HOH:O      | 1.86                     | 0.75              |
| 1:L:53[A]:GLU:HG2   | 5:L:4166:HOH:O      | 1.86                     | 0.75              |
| 1:G:27:ARG:HD3      | 1:G:58:ASP:O        | 1.85                     | 0.75              |
| 1:B:122:HIS:CD2     | 2:B:502:CMQ:H242    | 2.18                     | 0.75              |
| 1:E:77:TYR:OH       | 1:E:156:HIS:HE1     | 1.68                     | 0.75              |
| 1:G:3:VAL:HG11      | 1:G:18:ASP:HB2      | 1.68                     | 0.74              |
| 1:N:118:ARG:HG2     | 4:N:3007:GOL:H11    | 1.69                     | 0.74              |
| 1:K:104:THR:CG2     | 1:K:153:MET:CE      | 2.58                     | 0.74              |
| 1:C:22:ARG:HD2      | 5:C:4129:HOH:O      | 1.88                     | 0.73              |
| 1:L:5:MET:HA        | 1:L:17:PHE:O        | 1.89                     | 0.72              |
| 1:A:140:ARG:HG2     | 1:A:140:ARG:HH11    | 1.55                     | 0.72              |
| 1:B:178:GLU:HA      | 1:B:181:GLU:HG2     | 1.71                     | 0.72              |
| 1:M:15:ARG:HG2      | 1:M:15:ARG:HH21     | 1.55                     | 0.72              |
| 4:A:3001:GOL:H32    | 1:G:141:GLU:OE2     | 1.90                     | 0.71              |
| 5:A:4226:HOH:O      | 1:B:92[A]:MET:HE1   | 1.89                     | 0.71              |
| 1:M:116:ASN:HD21    | 1:N:148:ARG:NH1     | 1.88                     | 0.71              |
| 1:H:172:ARG:CD      | 5:H:4163:HOH:O      | 2.37                     | 0.71              |
| 1:J:193:ASN:H       | 1:J:193:ASN:ND2     | 1.86                     | 0.71              |
| 1:D:101:PHE:HA      | 1:D:153:MET:HE3     | 1.73                     | 0.71              |
| 1:B:143:LEU:HD11    | 1:I:136:GLU:CG      | 2.20                     | 0.70              |
| 1:I:122:HIS:CE1     | 2:I:509:CMQ:H241    | 2.25                     | 0.70              |
| 1:L:70:ILE:HG12     | 1:L:98[B]:MET:HE1   | 1.73                     | 0.70              |
| 1:E:141:GLU:OE2     | 4:F:3004:GOL:H32    | 1.91                     | 0.69              |
| 1:M:31[A]:LEU:HD13  | 1:M:39:MET:HE1      | 1.75                     | 0.69              |
| 1:C:122:HIS:CE1     | 2:C:503:CMQ:C24     | 2.75                     | 0.69              |
| 1:E:122:HIS:CE1     | 2:E:505:CMQ:H241    | 2.28                     | 0.69              |
| 1:H:172:ARG:HD2     | 5:H:4163:HOH:O      | 1.93                     | 0.69              |
| 1:I:122:HIS:CE1     | 2:I:509:CMQ:C24     | 2.74                     | 0.69              |
| 1:M:92[B]:MET:HB3   | 1:M:114:LEU:HD22    | 1.74                     | 0.69              |
| 1:B:10:THR:HG22     | 1:B:12:ARG:HG2      | 1.75                     | 0.68              |
| 1:I:153[A]:MET:HG2  | 1:I:164:ILE:HD12    | 1.74                     | 0.68              |
| 1:H:144:LYS:O       | 1:H:148:ARG:HG2     | 1.92                     | 0.68              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 3:K:4015:PGE:H22 | 5:K:4195:HOH:O      | 1.92                     | 0.68              |
| 1:J:166:ARG:HD3  | 5:J:4105:HOH:O      | 1.91                     | 0.68              |
| 1:E:38:HIS:HE1   | 5:E:4070:HOH:O      | 1.76                     | 0.68              |
| 1:E:15:ARG:CB    | 1:F:7:ILE:HG21      | 2.23                     | 0.68              |
| 1:F:140:ARG:NH1  | 5:F:4224:HOH:O      | 2.27                     | 0.68              |
| 1:H:153:MET:CE   | 1:H:184:LEU:HD21    | 2.23                     | 0.68              |
| 1:B:136:GLU:HB2  | 1:I:143:LEU:HD11    | 1.74                     | 0.67              |
| 1:J:166:ARG:CD   | 5:J:4105:HOH:O      | 2.41                     | 0.67              |
| 2:J:510:CMQ:H8   | 5:J:4155:HOH:O      | 1.92                     | 0.67              |
| 1:A:157:THR:CG2  | 1:A:184[B]:LEU:HD22 | 2.23                     | 0.67              |
| 1:A:182:TYR:CD2  | 1:A:184[B]:LEU:HD23 | 2.26                     | 0.67              |
| 1:L:162:GLU:HA   | 1:L:165:GLU:OE1     | 1.94                     | 0.67              |
| 1:A:140:ARG:HH11 | 1:A:140:ARG:CG      | 2.07                     | 0.67              |
| 4:C:3006:GOL:O3  | 1:D:118:ARG:CB      | 2.42                     | 0.67              |
| 1:E:122:HIS:CD2  | 2:E:505:CMQ:H242    | 2.20                     | 0.66              |
| 1:G:54:ASN:HD22  | 1:G:56:GLU:H        | 1.44                     | 0.66              |
| 1:G:135:ILE:HD13 | 1:N:142[B]:ILE:HD12 | 1.78                     | 0.66              |
| 1:C:122:HIS:CE1  | 2:C:503:CMQ:H241    | 2.31                     | 0.65              |
| 1:H:172:ARG:HH11 | 1:H:172:ARG:HG3     | 1.59                     | 0.65              |
| 1:C:31:LEU:HD13  | 1:C:39:MET:HE1      | 1.79                     | 0.65              |
| 1:D:7:ILE:O      | 1:D:8:GLU:HB2       | 1.95                     | 0.65              |
| 1:F:5:MET:HE2    | 1:F:16:SER:OG       | 1.97                     | 0.65              |
| 1:L:161:LEU:O    | 1:L:165:GLU:HG3     | 1.95                     | 0.65              |
| 1:J:193:ASN:H    | 1:J:193:ASN:HD22    | 1.45                     | 0.64              |
| 1:L:2:LEU:HD22   | 1:M:3:VAL:HG21      | 1.80                     | 0.64              |
| 1:C:136:GLU:O    | 1:C:140[B]:ARG:HG2  | 1.98                     | 0.64              |
| 1:I:18:ASP:OD2   | 1:I:21:SER:OG       | 2.09                     | 0.64              |
| 1:E:70:ILE:HD12  | 2:E:505:CMQ:H22A    | 1.78                     | 0.64              |
| 1:M:2:LEU:HD21   | 5:N:4097:HOH:O      | 1.96                     | 0.64              |
| 1:N:173:PHE:HE1  | 4:N:3007:GOL:H31    | 1.63                     | 0.64              |
| 4:C:3006:GOL:H12 | 5:C:4108:HOH:O      | 1.97                     | 0.64              |
| 1:D:77:TYR:OH    | 1:D:156:HIS:HE1     | 1.81                     | 0.64              |
| 1:H:31:LEU:HD13  | 1:H:39:MET:HE1      | 1.79                     | 0.64              |
| 1:B:104:THR:HB   | 1:B:184:LEU:HD23    | 1.78                     | 0.64              |
| 1:K:153:MET:HA   | 1:K:153:MET:HE2     | 1.78                     | 0.64              |
| 1:I:111:ARG:O    | 1:I:185[B]:VAL:HG23 | 1.97                     | 0.64              |
| 1:J:116:ASN:ND2  | 1:K:148:ARG:HH11    | 1.95                     | 0.64              |
| 1:A:144:LYS:HE2  | 5:A:4099:HOH:O      | 1.97                     | 0.63              |
| 1:A:143:LEU:HG   | 5:A:4180:HOH:O      | 1.98                     | 0.63              |
| 1:K:17:PHE:CE2   | 1:K:25:LYS:HE3      | 2.33                     | 0.63              |
| 1:N:173:PHE:CE1  | 4:N:3007:GOL:H31    | 2.32                     | 0.63              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:D:22:ARG:HD2     | 1:D:22:ARG:O        | 1.97                     | 0.63              |
| 1:L:98[B]:MET:HE2  | 2:L:512:CMQ:H171    | 1.79                     | 0.62              |
| 1:A:153[A]:MET:HE2 | 5:A:4086:HOH:O      | 1.98                     | 0.62              |
| 1:B:10:THR:HB      | 1:B:13:GLY:O        | 1.99                     | 0.62              |
| 1:D:122:HIS:CE1    | 2:D:504:CMQ:H241    | 2.34                     | 0.62              |
| 1:A:77:TYR:OH      | 1:A:156:HIS:HE1     | 1.81                     | 0.62              |
| 1:J:31:LEU:HD13    | 1:J:39:MET:HE1      | 1.81                     | 0.62              |
| 1:C:5:MET:HG3      | 1:C:5:MET:O         | 1.99                     | 0.62              |
| 1:A:148:ARG:HH11   | 1:B:116:ASN:ND2     | 1.97                     | 0.62              |
| 1:E:156:HIS:HD2    | 5:E:4016:HOH:O      | 1.81                     | 0.62              |
| 1:E:92:MET:HB3     | 1:E:114:LEU:HD22    | 1.82                     | 0.62              |
| 1:G:136:GLU:OE1    | 1:G:140:ARG:NH1     | 2.31                     | 0.62              |
| 1:J:70:ILE:HA      | 1:J:98:MET:HE3      | 1.82                     | 0.62              |
| 1:L:2:LEU:HD23     | 5:M:4111:HOH:O      | 1.99                     | 0.61              |
| 1:B:181:GLU:HG3    | 5:B:4080:HOH:O      | 1.98                     | 0.61              |
| 1:J:176:ALA:HB1    | 1:J:188:ILE:HD12    | 1.81                     | 0.61              |
| 1:M:104:THR:CB     | 1:M:184[B]:LEU:HD12 | 2.29                     | 0.61              |
| 1:F:41:ASN:ND2     | 1:G:32:THR:OG1      | 2.32                     | 0.61              |
| 1:M:116:ASN:ND2    | 1:N:148:ARG:HH11    | 1.99                     | 0.61              |
| 1:L:70:ILE:HG12    | 1:L:98[B]:MET:CE    | 2.31                     | 0.60              |
| 1:G:25:LYS:NZ      | 5:G:4237:HOH:O      | 2.34                     | 0.60              |
| 1:H:17:PHE:HD2     | 1:H:21:SER:HB3      | 1.66                     | 0.60              |
| 1:J:114:LEU:HG     | 1:K:78:ASP:HB3      | 1.82                     | 0.60              |
| 1:D:122:HIS:NE2    | 2:D:504:CMQ:H241    | 2.09                     | 0.60              |
| 2:E:505:CMQ:C6     | 5:E:4152:HOH:O      | 2.46                     | 0.60              |
| 1:E:5:MET:HE3      | 1:E:16:SER:HB3      | 1.83                     | 0.60              |
| 1:B:70:ILE:HD12    | 2:B:502:CMQ:H21A    | 1.82                     | 0.59              |
| 1:D:140:ARG:HD3    | 5:D:4160:HOH:O      | 2.01                     | 0.59              |
| 1:E:144[A]:LYS:HD3 | 5:F:4191:HOH:O      | 2.03                     | 0.59              |
| 1:H:96:ALA:HB1     | 1:H:120:MET:HE2     | 1.83                     | 0.59              |
| 1:M:116:ASN:ND2    | 1:N:148:ARG:NH1     | 2.50                     | 0.59              |
| 1:J:116:ASN:HD21   | 1:K:148:ARG:HH11    | 1.49                     | 0.59              |
| 1:J:116:ASN:HD21   | 1:K:148:ARG:NH1     | 2.00                     | 0.59              |
| 1:B:31:LEU:HD13    | 1:B:39:MET:HE1      | 1.85                     | 0.59              |
| 1:B:178:GLU:O      | 1:B:181:GLU:HG2     | 2.02                     | 0.59              |
| 5:J:4045:HOH:O     | 2:K:511:CMQ:H4      | 2.03                     | 0.59              |
| 1:B:178:GLU:HA     | 1:B:181:GLU:CD      | 2.28                     | 0.59              |
| 1:E:38:HIS:HD2     | 5:E:4103:HOH:O      | 1.85                     | 0.59              |
| 3:K:4015:PGE:H5    | 5:K:4195:HOH:O      | 2.02                     | 0.59              |
| 1:M:161:LEU:O      | 1:M:165:GLU:HG3     | 2.03                     | 0.59              |
| 1:F:42:LEU:HD11    | 1:G:3:VAL:HG13      | 1.83                     | 0.59              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:A:104:THR:CG2     | 1:A:153[B]:MET:CE   | 2.79                     | 0.59              |
| 1:H:4:PRO:CD        | 1:I:42:LEU:HD11     | 2.32                     | 0.58              |
| 1:H:34:GLN:HE21     | 1:H:68:GLY:HA2      | 1.67                     | 0.58              |
| 1:A:5:MET:HE3       | 1:A:16:SER:OG       | 2.03                     | 0.58              |
| 1:A:34:GLN:OE1      | 1:A:68:GLY:HA2      | 2.03                     | 0.58              |
| 1:I:70:ILE:HD12     | 2:I:509:CMQ:H21A    | 1.85                     | 0.58              |
| 1:I:32:THR:OG1      | 1:J:41:ASN:ND2      | 2.36                     | 0.58              |
| 1:B:178:GLU:HA      | 1:B:181:GLU:CG      | 2.33                     | 0.58              |
| 1:J:145:VAL:HG21    | 2:J:510:CMQ:H5      | 1.86                     | 0.58              |
| 1:B:38:HIS:HE1      | 5:C:4132:HOH:O      | 1.86                     | 0.58              |
| 1:D:70:ILE:HD12     | 2:D:504:CMQ:H22A    | 1.86                     | 0.58              |
| 1:B:114[B]:LEU:HD22 | 1:B:189:LEU:HB2     | 1.86                     | 0.58              |
| 1:B:129:GLN:HG2     | 5:B:4168:HOH:O      | 2.03                     | 0.58              |
| 1:J:7:ILE:HG12      | 1:J:16:SER:HA       | 1.85                     | 0.58              |
| 5:A:4226:HOH:O      | 1:B:92[A]:MET:CE    | 2.50                     | 0.57              |
| 1:M:70:ILE:HD12     | 2:M:513:CMQ:H21A    | 1.86                     | 0.57              |
| 1:M:98[A]:MET:HE1   | 1:M:149:MET:HE1     | 1.86                     | 0.57              |
| 1:D:101:PHE:CD1     | 1:D:153:MET:HE3     | 2.39                     | 0.57              |
| 1:L:4:PRO:HD3       | 1:M:42:LEU:HD11     | 1.87                     | 0.57              |
| 1:D:22:ARG:O        | 1:D:25:LYS:HB2      | 2.04                     | 0.57              |
| 1:K:70:ILE:HA       | 1:K:98:MET:HE3      | 1.86                     | 0.57              |
| 1:E:31:LEU:HD13     | 1:E:39:MET:HE1      | 1.87                     | 0.57              |
| 1:J:34:GLN:HE21     | 1:J:68:GLY:HA2      | 1.69                     | 0.57              |
| 1:K:92:MET:HE1      | 5:L:4228:HOH:O      | 2.05                     | 0.57              |
| 1:A:108:LYS:HE2     | 1:A:186:ASP:OD1     | 2.05                     | 0.57              |
| 1:J:136[B]:GLU:OE2  | 1:J:140:ARG:NH1     | 2.36                     | 0.57              |
| 1:H:27:ARG:HD3      | 1:H:57:LYS:HE2      | 1.86                     | 0.56              |
| 1:M:34[A]:GLN:HG2   | 5:M:4144:HOH:O      | 2.05                     | 0.56              |
| 1:K:92:MET:CE       | 5:L:4228:HOH:O      | 2.53                     | 0.56              |
| 1:A:140:ARG:CG      | 1:A:140:ARG:NH1     | 2.68                     | 0.56              |
| 1:C:70:ILE:HD12     | 2:C:503:CMQ:H21A    | 1.86                     | 0.56              |
| 1:D:115:PRO:HD3     | 1:D:189:LEU:O       | 2.05                     | 0.56              |
| 1:L:140:ARG:HG3     | 5:L:4252:HOH:O      | 2.04                     | 0.56              |
| 1:D:119:VAL:HG11    | 1:D:184:LEU:HD13    | 1.87                     | 0.56              |
| 1:C:41:ASN:ND2      | 1:D:32:THR:OG1      | 2.39                     | 0.56              |
| 1:I:96:ALA:HB1      | 1:I:120[B]:MET:HE3  | 1.88                     | 0.56              |
| 1:L:70:ILE:HA       | 1:L:98[B]:MET:CE    | 2.36                     | 0.56              |
| 1:L:172:ARG:NH2     | 5:L:4024:HOH:O      | 2.36                     | 0.56              |
| 1:I:111:ARG:C       | 1:I:185[B]:VAL:HG23 | 2.31                     | 0.56              |
| 1:D:104:THR:CG2     | 1:D:153:MET:HE1     | 2.36                     | 0.55              |
| 1:H:4:PRO:HD2       | 1:I:42:LEU:HD11     | 1.89                     | 0.55              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:C:153:MET:HE2     | 5:C:4090:HOH:O     | 2.06                     | 0.55              |
| 1:H:120:MET:HE3     | 1:H:120:MET:C      | 2.31                     | 0.55              |
| 1:A:73:GLY:HA3      | 1:A:98[B]:MET:SD   | 2.47                     | 0.55              |
| 1:B:18:ASP:HB3      | 1:C:5:MET:HG2      | 1.88                     | 0.55              |
| 1:B:127:GLY:HA3     | 1:I:129:GLN:HG3    | 1.88                     | 0.55              |
| 1:G:129[A]:GLN:HG2  | 1:N:127:GLY:HA3    | 1.89                     | 0.55              |
| 1:A:74:MET:SD       | 1:A:98[A]:MET:HE1  | 2.47                     | 0.55              |
| 1:M:189:LEU:HD11    | 3:M:4013:PGE:H3    | 1.89                     | 0.55              |
| 1:L:70:ILE:HA       | 1:L:98[B]:MET:HE3  | 1.88                     | 0.54              |
| 1:A:104:THR:CG2     | 1:A:153[B]:MET:HE1 | 2.36                     | 0.54              |
| 1:D:148:ARG:NH2     | 1:E:116:ASN:HD21   | 2.00                     | 0.54              |
| 1:K:191:HIS:CE1     | 1:L:81[A]:GLN:HG3  | 2.42                     | 0.54              |
| 4:C:3006:GOL:C1     | 5:C:4108:HOH:O     | 2.54                     | 0.54              |
| 1:H:172:ARG:HH11    | 1:H:172:ARG:HG2    | 1.71                     | 0.54              |
| 1:A:122:HIS:CD2     | 2:A:501:CMQ:H242   | 2.26                     | 0.53              |
| 1:C:55:PRO:HB2      | 1:C:84:LYS:HG3     | 1.90                     | 0.53              |
| 1:A:122:HIS:NE2     | 2:A:501:CMQ:C16    | 2.66                     | 0.53              |
| 1:H:153:MET:HE1     | 1:H:184:LEU:HD21   | 1.89                     | 0.53              |
| 1:I:27:ARG:HD3      | 1:I:58:ASP:O       | 2.09                     | 0.53              |
| 1:D:129[B]:GLN:NE2  | 5:D:4145:HOH:O     | 2.26                     | 0.53              |
| 1:E:57:LYS:O        | 1:E:85:PRO:HB3     | 2.09                     | 0.53              |
| 1:G:153[B]:MET:HE1  | 1:G:184:LEU:HD21   | 1.91                     | 0.53              |
| 1:M:73:GLY:HA3      | 1:M:98[B]:MET:HE2  | 1.90                     | 0.53              |
| 1:A:189[A]:LEU:HD13 | 1:G:82:PHE:CE1     | 2.43                     | 0.53              |
| 1:I:27:ARG:NH2      | 1:I:50:LEU:O       | 2.39                     | 0.53              |
| 1:C:174[A]:LEU:HD12 | 1:C:184:LEU:HD12   | 1.91                     | 0.53              |
| 1:G:3:VAL:CG1       | 1:G:19:ILE:HG22    | 2.39                     | 0.53              |
| 1:J:6:VAL:HG21      | 1:J:22:ARG:HG2     | 1.90                     | 0.53              |
| 1:L:143:LEU:HG      | 5:L:4183:HOH:O     | 2.09                     | 0.53              |
| 1:A:189[B]:LEU:HD22 | 1:G:82:PHE:HE1     | 1.74                     | 0.52              |
| 1:G:54:ASN:HD22     | 1:G:54:ASN:C       | 2.16                     | 0.52              |
| 1:B:148[A]:ARG:NH1  | 1:C:116:ASN:ND2    | 2.41                     | 0.52              |
| 1:G:3:VAL:CB        | 1:G:18:ASP:HB2     | 2.39                     | 0.52              |
| 1:A:136:GLU:O       | 1:A:140:ARG:HD3    | 2.09                     | 0.52              |
| 1:I:34:GLN:NE2      | 1:I:68:GLY:HA2     | 2.24                     | 0.52              |
| 1:J:122:HIS:CE1     | 2:J:510:CMQ:H241   | 2.41                     | 0.52              |
| 3:N:4014:PGE:H6     | 5:N:4132:HOH:O     | 2.09                     | 0.52              |
| 1:G:54:ASN:ND2      | 1:G:56:GLU:H       | 2.07                     | 0.52              |
| 1:M:92[A]:MET:HB3   | 1:M:114:LEU:HD22   | 1.91                     | 0.52              |
| 1:A:148:ARG:HD3     | 1:B:116:ASN:ND2    | 2.25                     | 0.52              |
| 1:C:84:LYS:CD       | 1:D:192:ARG:HG2    | 2.39                     | 0.52              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 1:D:101:PHE:HA      | 1:D:153:MET:HE1   | 1.91                     | 0.52              |
| 1:E:15:ARG:CB       | 1:F:7:ILE:CG2     | 2.88                     | 0.52              |
| 1:J:8:GLU:OE2       | 1:J:22:ARG:NE     | 2.42                     | 0.51              |
| 1:J:189:LEU:HD11    | 3:J:4010:PGE:H22  | 1.91                     | 0.51              |
| 1:I:57:LYS:O        | 1:I:85:PRO:HB3    | 2.09                     | 0.51              |
| 1:J:122:HIS:CD2     | 2:J:510:CMQ:H242  | 2.23                     | 0.51              |
| 1:E:62:TYR:CD2      | 1:E:92:MET:HE3    | 2.45                     | 0.51              |
| 1:G:118:ARG:HB2     | 4:G:3009:GOL:H11  | 1.92                     | 0.51              |
| 1:L:57:LYS:NZ       | 5:L:4090:HOH:O    | 2.43                     | 0.51              |
| 1:N:142[B]:ILE:HG12 | 2:N:514:CMQ:C7    | 2.40                     | 0.51              |
| 1:D:167:ASP:HA      | 1:D:172:ARG:HH21  | 1.75                     | 0.51              |
| 1:E:9:GLN:HA        | 1:E:14:GLU:HG2    | 1.91                     | 0.51              |
| 1:F:38:HIS:HD2      | 5:F:4166:HOH:O    | 1.91                     | 0.51              |
| 1:J:147:GLY:O       | 1:J:151:GLU:HG3   | 2.10                     | 0.51              |
| 1:I:54:ASN:CG       | 1:I:57:LYS:HG3    | 2.36                     | 0.51              |
| 1:H:32:THR:OG1      | 1:I:41:ASN:ND2    | 2.44                     | 0.51              |
| 1:F:148:ARG:NH1     | 1:G:116:ASN:OD1   | 2.37                     | 0.51              |
| 1:K:124:PRO:HD3     | 2:K:511:CMQ:H22   | 1.92                     | 0.51              |
| 1:C:22:ARG:HH11     | 1:C:22:ARG:CB     | 2.13                     | 0.51              |
| 1:E:14:GLU:N        | 5:E:4196:HOH:O    | 2.43                     | 0.51              |
| 1:N:62:TYR:CD2      | 1:N:92:MET:HE3    | 2.46                     | 0.50              |
| 1:A:189[A]:LEU:HD11 | 3:A:4001:PGE:H5   | 1.93                     | 0.50              |
| 1:D:101:PHE:HD1     | 1:D:153:MET:HE3   | 1.75                     | 0.50              |
| 1:M:92[A]:MET:HE1   | 5:N:4043:HOH:O    | 2.10                     | 0.50              |
| 1:H:34:GLN:HE21     | 1:H:68:GLY:CA     | 2.23                     | 0.50              |
| 1:A:92:MET:HB3      | 1:A:114:LEU:HD22  | 1.94                     | 0.50              |
| 1:K:191:HIS:HE1     | 1:L:81[A]:GLN:HG3 | 1.77                     | 0.50              |
| 1:M:98[A]:MET:HE1   | 1:M:149:MET:CE    | 2.42                     | 0.50              |
| 1:A:108:LYS:HD3     | 5:A:4139:HOH:O    | 2.12                     | 0.50              |
| 1:L:136[B]:GLU:OE1  | 1:L:140:ARG:NH1   | 2.41                     | 0.50              |
| 1:F:57:LYS:O        | 1:F:85:PRO:HB3    | 2.12                     | 0.49              |
| 1:H:4:PRO:HD3       | 1:I:42:LEU:HD11   | 1.94                     | 0.49              |
| 1:B:10:THR:HG22     | 1:B:10:THR:O      | 2.11                     | 0.49              |
| 1:A:32:THR:OG1      | 1:G:41:ASN:ND2    | 2.46                     | 0.49              |
| 1:G:147:GLY:O       | 1:G:151:GLU:HG3   | 2.12                     | 0.49              |
| 1:H:27:ARG:CD       | 1:H:57:LYS:HE2    | 2.42                     | 0.49              |
| 1:M:31[B]:LEU:HG    | 1:M:43:ILE:CD1    | 2.42                     | 0.49              |
| 1:A:118:ARG:HB3     | 4:A:3001:GOL:O3   | 2.12                     | 0.49              |
| 1:A:54:ASN:HD22     | 1:A:56:GLU:H      | 1.60                     | 0.49              |
| 1:L:4:PRO:O         | 1:L:18:ASP:HA     | 2.12                     | 0.49              |
| 1:D:104:THR:HG22    | 1:D:153:MET:HE1   | 1.95                     | 0.49              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:I:192:ARG:HG3    | 1:I:193:ASN:N       | 2.27                     | 0.49              |
| 1:G:56:GLU:HG3     | 5:G:4223:HOH:O      | 2.12                     | 0.49              |
| 1:H:42[A]:LEU:HD11 | 1:N:4:PRO:CD        | 2.43                     | 0.49              |
| 1:H:5:MET:HG3      | 1:I:21:SER:OG       | 2.13                     | 0.48              |
| 1:I:153[B]:MET:HE1 | 1:I:184:LEU:CD2     | 2.37                     | 0.48              |
| 1:J:55:PRO:HB3     | 1:J:84:LYS:HE3      | 1.95                     | 0.48              |
| 1:A:92:MET:CE      | 5:G:4106:HOH:O      | 2.51                     | 0.48              |
| 1:E:9:GLN:HG3      | 1:E:14:GLU:OE2      | 2.13                     | 0.48              |
| 1:I:98[B]:MET:HE1  | 1:I:149:MET:HE1     | 1.94                     | 0.48              |
| 1:I:115:PRO:HD3    | 1:I:189:LEU:O       | 2.13                     | 0.48              |
| 1:K:141:GLU:HG3    | 2:K:511:CMQ:H5      | 1.94                     | 0.48              |
| 1:N:70:ILE:HD12    | 2:N:514:CMQ:H22A    | 1.95                     | 0.48              |
| 1:B:41:ASN:ND2     | 1:C:32:THR:OG1      | 2.47                     | 0.48              |
| 1:C:84:LYS:NZ      | 1:D:193:ASN:HD21    | 2.11                     | 0.48              |
| 1:D:104:THR:HG21   | 1:D:153:MET:CE      | 2.43                     | 0.48              |
| 1:D:129[A]:GLN:NE2 | 1:D:130:GLY:N       | 2.61                     | 0.48              |
| 1:F:17:PHE:CE1     | 1:G:6:VAL:HG13      | 2.48                     | 0.48              |
| 1:J:166:ARG:HD2    | 5:J:4105:HOH:O      | 2.10                     | 0.48              |
| 1:I:80:MET:HE1     | 1:I:105:ALA:HB3     | 1.94                     | 0.48              |
| 1:K:92:MET:HB3     | 1:K:114[B]:LEU:HD22 | 1.93                     | 0.48              |
| 1:M:92[A]:MET:CE   | 5:N:4043:HOH:O      | 2.60                     | 0.48              |
| 1:B:18:ASP:HB3     | 1:C:5:MET:CG        | 2.43                     | 0.48              |
| 1:F:38:HIS:HE1     | 5:G:4058:HOH:O      | 1.95                     | 0.48              |
| 1:A:123:GLN:HE22   | 1:H:133:THR:H       | 1.60                     | 0.48              |
| 1:D:7:ILE:O        | 1:D:8:GLU:CB        | 2.62                     | 0.48              |
| 1:D:104:THR:CG2    | 1:D:153:MET:CE      | 2.92                     | 0.48              |
| 4:H:3008:GOL:H31   | 1:I:141:GLU:OE2     | 2.14                     | 0.48              |
| 2:A:501:CMQ:H7     | 5:A:4174:HOH:O      | 2.14                     | 0.48              |
| 1:B:22:ARG:O       | 1:B:25[A]:LYS:HG2   | 2.13                     | 0.48              |
| 1:B:153[B]:MET:HG3 | 5:B:4129:HOH:O      | 2.13                     | 0.48              |
| 1:E:51:GLU:HG3     | 1:E:85:PRO:HD3      | 1.96                     | 0.48              |
| 1:D:3:VAL:HG11     | 1:E:2:LEU:HD22      | 1.96                     | 0.47              |
| 1:C:148:ARG:NH2    | 1:C:151:GLU:OE1     | 2.47                     | 0.47              |
| 1:K:41:ASN:ND2     | 5:K:4058:HOH:O      | 2.46                     | 0.47              |
| 1:G:3:VAL:HG13     | 1:G:19:ILE:HG22     | 1.95                     | 0.47              |
| 1:G:3:VAL:HB       | 1:G:18:ASP:HB2      | 1.96                     | 0.47              |
| 3:F:4006:PGE:H4    | 5:F:4103:HOH:O      | 2.14                     | 0.47              |
| 1:G:27:ARG:CD      | 1:G:58:ASP:O        | 2.60                     | 0.47              |
| 1:C:84:LYS:HD2     | 1:D:192:ARG:HG2     | 1.97                     | 0.47              |
| 2:L:512:CMQ:C13    | 5:L:4248:HOH:O      | 2.61                     | 0.47              |
| 1:K:62:TYR:CD2     | 1:K:92:MET:HE3      | 2.50                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C:144:LYS:HE3    | 5:C:4030:HOH:O     | 2.14                     | 0.47              |
| 1:L:5:MET:HE3      | 1:L:17:PHE:HD1     | 1.80                     | 0.47              |
| 1:E:3:VAL:HG12     | 1:E:18:ASP:HB2     | 1.97                     | 0.47              |
| 1:C:5:MET:HB2      | 1:C:16:SER:HB3     | 1.97                     | 0.47              |
| 1:I:98[B]:MET:HE1  | 1:I:149:MET:CE     | 2.44                     | 0.47              |
| 1:D:148:ARG:HE     | 1:E:116:ASN:ND2    | 2.13                     | 0.46              |
| 1:K:23:LEU:HD11    | 1:L:49:PHE:HB2     | 1.97                     | 0.46              |
| 1:L:70:ILE:HD12    | 2:L:512:CMQ:H21A   | 1.97                     | 0.46              |
| 1:B:143:LEU:CD1    | 1:I:136:GLU:HG3    | 2.42                     | 0.46              |
| 1:M:6:VAL:HG12     | 1:M:7:ILE:N        | 2.30                     | 0.46              |
| 1:M:190:THR:HB     | 5:M:4264:HOH:O     | 2.14                     | 0.46              |
| 1:N:192:ARG:HH12   | 3:N:4014:PGE:H5    | 1.81                     | 0.46              |
| 1:B:163:GLN:HE22   | 1:B:166[B]:ARG:NH2 | 2.09                     | 0.46              |
| 1:N:31[A]:LEU:HD13 | 1:N:39:MET:HE1     | 1.98                     | 0.46              |
| 1:B:192:ARG:NH1    | 3:B:4002:PGE:H42   | 2.31                     | 0.46              |
| 1:A:22:ARG:O       | 1:A:25:LYS:HG2     | 2.16                     | 0.46              |
| 1:E:114:LEU:O      | 1:E:117:SER:HB2    | 2.16                     | 0.46              |
| 1:H:172:ARG:CG     | 1:H:172:ARG:NH1    | 2.62                     | 0.46              |
| 1:D:148:ARG:HH21   | 1:E:116:ASN:ND2    | 2.05                     | 0.46              |
| 1:K:89:THR:C       | 1:K:90:ILE:HG13    | 2.41                     | 0.46              |
| 1:C:84:LYS:HG2     | 1:C:85:PRO:HD3     | 1.97                     | 0.45              |
| 5:D:4141:HOH:O     | 1:E:2:LEU:HD23     | 2.15                     | 0.45              |
| 1:E:19:ILE:HD12    | 1:E:19:ILE:HA      | 1.81                     | 0.45              |
| 1:E:123:GLN:HE22   | 1:L:133:THR:H      | 1.64                     | 0.45              |
| 1:L:144:LYS:NZ     | 5:L:4101:HOH:O     | 2.31                     | 0.45              |
| 1:K:36:GLU:CD      | 1:K:38:HIS:H       | 2.25                     | 0.45              |
| 1:D:31:LEU:HD13    | 1:D:39:MET:HE1     | 1.97                     | 0.45              |
| 1:H:4:PRO:HD3      | 1:I:42:LEU:HD21    | 1.99                     | 0.45              |
| 1:J:136[B]:GLU:HG2 | 1:J:140:ARG:HD3    | 1.98                     | 0.45              |
| 1:A:82:PHE:CE1     | 1:B:192:ARG:HA     | 2.51                     | 0.45              |
| 1:A:108:LYS:NZ     | 5:A:4221:HOH:O     | 2.49                     | 0.45              |
| 1:D:22:ARG:HD2     | 1:D:22:ARG:C       | 2.41                     | 0.45              |
| 1:G:3:VAL:O        | 1:G:5:MET:HG2      | 2.16                     | 0.45              |
| 1:M:92[A]:MET:HE1  | 1:N:44:VAL:HG11    | 1.97                     | 0.45              |
| 1:M:104:THR:HG21   | 1:M:153:MET:HE2    | 1.97                     | 0.45              |
| 1:H:97:SER:HB2     | 1:H:120:MET:HE1    | 1.98                     | 0.45              |
| 1:H:120:MET:HE3    | 1:H:120:MET:O      | 2.17                     | 0.45              |
| 1:B:23:LEU:HD23    | 1:B:23:LEU:HA      | 1.82                     | 0.45              |
| 1:D:31:LEU:HB2     | 1:D:43:ILE:HD13    | 1.99                     | 0.45              |
| 1:J:51:GLU:HG3     | 1:J:85:PRO:HD3     | 1.99                     | 0.45              |
| 4:K:3010:GOL:H11   | 1:L:141:GLU:OE2    | 2.16                     | 0.45              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:M:140:ARG:NH2     | 5:M:4254:HOH:O     | 2.44                     | 0.45              |
| 1:B:10:THR:C        | 1:B:12:ARG:H       | 2.26                     | 0.45              |
| 1:C:3:VAL:HA        | 5:C:4140:HOH:O     | 2.17                     | 0.45              |
| 1:I:96:ALA:HB1      | 1:I:120[A]:MET:HE2 | 1.99                     | 0.45              |
| 1:D:104:THR:HG21    | 1:D:153:MET:HE1    | 1.99                     | 0.44              |
| 1:H:172:ARG:HG2     | 1:H:172:ARG:NH1    | 2.32                     | 0.44              |
| 1:J:116:ASN:HD22    | 1:K:148:ARG:HD3    | 1.82                     | 0.44              |
| 1:E:38:HIS:CE1      | 5:E:4070:HOH:O     | 2.61                     | 0.44              |
| 1:F:147:GLY:O       | 1:F:151:GLU:HG3    | 2.18                     | 0.44              |
| 1:G:3:VAL:HG12      | 1:G:19:ILE:H       | 1.83                     | 0.44              |
| 1:B:192:ARG:HH12    | 3:B:4002:PGE:H42   | 1.83                     | 0.44              |
| 1:B:96:ALA:HB1      | 1:B:120[A]:MET:HE3 | 1.99                     | 0.44              |
| 1:H:17:PHE:HB3      | 1:H:21:SER:HB2     | 2.00                     | 0.44              |
| 1:A:70:ILE:HA       | 1:A:98[B]:MET:HE3  | 2.00                     | 0.44              |
| 1:I:172:ARG:HD3     | 5:I:4062:HOH:O     | 2.16                     | 0.44              |
| 1:K:104:THR:HG21    | 1:K:153:MET:HE2    | 1.90                     | 0.44              |
| 1:A:156:HIS:HD2     | 5:A:4007:HOH:O     | 1.99                     | 0.44              |
| 1:I:170[B]:ARG:HE   | 1:I:170[B]:ARG:HB3 | 1.39                     | 0.44              |
| 1:M:153:MET:HE3     | 1:M:153:MET:HB2    | 1.68                     | 0.44              |
| 1:H:172:ARG:NE      | 5:H:4163:HOH:O     | 2.51                     | 0.44              |
| 1:I:185[B]:VAL:HG22 | 1:I:186:ASP:N      | 2.32                     | 0.44              |
| 2:I:509:CMQ:H7      | 5:I:4126:HOH:O     | 2.17                     | 0.44              |
| 1:M:34[A]:GLN:NE2   | 1:M:68:GLY:HA2     | 2.32                     | 0.43              |
| 1:M:176:ALA:HB1     | 1:M:188[B]:ILE:CD1 | 2.47                     | 0.43              |
| 1:B:144:LYS:O       | 1:B:148[B]:ARG:HG2 | 2.18                     | 0.43              |
| 1:C:42[B]:LEU:HD11  | 1:D:4:PRO:HD3      | 2.00                     | 0.43              |
| 1:I:70:ILE:O        | 1:I:74:MET:HG2     | 2.19                     | 0.43              |
| 1:L:190:THR:HG22    | 1:L:191:HIS:CD2    | 2.54                     | 0.43              |
| 1:C:15:ARG:NH1      | 1:C:15:ARG:CG      | 2.56                     | 0.43              |
| 1:C:133:THR:H       | 1:J:123:GLN:HE22   | 1.66                     | 0.43              |
| 1:A:70:ILE:HD12     | 2:A:501:CMQ:H21A   | 2.00                     | 0.43              |
| 1:D:31:LEU:HB2      | 1:D:43:ILE:CD1     | 2.48                     | 0.43              |
| 1:D:136:GLU:CD      | 1:D:140:ARG:NH2    | 2.77                     | 0.43              |
| 1:L:25:LYS:HA       | 5:L:4198:HOH:O     | 2.17                     | 0.43              |
| 1:B:10:THR:O        | 1:B:10:THR:CG2     | 2.67                     | 0.43              |
| 1:E:115:PRO:HD3     | 1:E:189:LEU:O      | 2.19                     | 0.43              |
| 1:F:136[A]:GLU:OE2  | 5:F:4185:HOH:O     | 2.21                     | 0.43              |
| 1:C:23:LEU:HD12     | 1:C:30:PHE:HE2     | 1.83                     | 0.43              |
| 1:D:101:PHE:CD1     | 1:D:153:MET:CE     | 3.02                     | 0.43              |
| 1:B:123:GLN:HE22    | 1:I:133:THR:H      | 1.67                     | 0.43              |
| 1:G:133:THR:H       | 1:N:123:GLN:HE22   | 1.67                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:M:34[A]:GLN:CD    | 1:M:68:GLY:HA2      | 2.43                     | 0.43              |
| 1:E:3:VAL:CG1       | 1:E:18:ASP:HB2      | 2.49                     | 0.43              |
| 1:E:153:MET:HE2     | 5:E:4193:HOH:O      | 2.08                     | 0.43              |
| 1:F:129:GLN:OE1     | 1:M:127:GLY:HA3     | 2.18                     | 0.43              |
| 1:K:4:PRO:HD3       | 1:L:42:LEU:HD21     | 2.00                     | 0.43              |
| 1:K:57:LYS:O        | 1:K:85:PRO:HB3      | 2.19                     | 0.43              |
| 1:M:176:ALA:HB1     | 1:M:188[B]:ILE:HD12 | 2.00                     | 0.43              |
| 1:N:73:GLY:HA3      | 1:N:98[B]:MET:HE2   | 2.01                     | 0.43              |
| 1:A:189[B]:LEU:HD22 | 1:G:82:PHE:CE1      | 2.53                     | 0.43              |
| 1:D:70:ILE:HD12     | 2:D:504:CMQ:C2      | 2.48                     | 0.43              |
| 1:B:176:ALA:HB3     | 1:B:177:PRO:HD3     | 2.00                     | 0.42              |
| 1:C:23:LEU:HD12     | 1:C:30:PHE:CE2      | 2.54                     | 0.42              |
| 1:K:31:LEU:C        | 1:K:31:LEU:HD23     | 2.44                     | 0.42              |
| 1:M:3:VAL:HG13      | 1:M:19:ILE:HG22     | 2.01                     | 0.42              |
| 1:N:62:TYR:HD2      | 1:N:92:MET:HE3      | 1.84                     | 0.42              |
| 4:H:3008:GOL:H11    | 5:H:4135:HOH:O      | 2.20                     | 0.42              |
| 1:K:104:THR:HG22    | 1:K:153:MET:HE1     | 1.89                     | 0.42              |
| 1:C:174[A]:LEU:HD23 | 5:C:4076:HOH:O      | 2.20                     | 0.42              |
| 1:K:115:PRO:HD3     | 1:K:189:LEU:O       | 2.19                     | 0.42              |
| 1:K:153:MET:CE      | 1:K:153:MET:HA      | 2.48                     | 0.42              |
| 1:B:178:GLU:CA      | 1:B:181:GLU:HG2     | 2.44                     | 0.42              |
| 1:I:176:ALA:HB3     | 1:I:177:PRO:HD3     | 2.00                     | 0.42              |
| 1:L:5:MET:O         | 1:M:21:SER:HB3      | 2.19                     | 0.42              |
| 1:E:35:VAL:C        | 1:E:36:GLU:HG2      | 2.42                     | 0.42              |
| 1:F:123:GLN:HE22    | 1:M:133:THR:H       | 1.67                     | 0.42              |
| 1:I:73:GLY:HA3      | 1:I:98[A]:MET:HE2   | 2.00                     | 0.42              |
| 1:J:145:VAL:O       | 1:J:149:MET:HG2     | 2.20                     | 0.42              |
| 1:L:143:LEU:CG      | 5:L:4183:HOH:O      | 2.66                     | 0.42              |
| 2:L:512:CMQ:H133    | 2:L:512:CMQ:N1      | 2.35                     | 0.42              |
| 1:C:41:ASN:HD21     | 1:D:30:PHE:HB3      | 1.84                     | 0.42              |
| 1:D:124:PRO:HA      | 2:D:504:CMQ:O3      | 2.19                     | 0.42              |
| 1:G:4:PRO:O         | 1:G:18:ASP:HA       | 2.19                     | 0.42              |
| 1:H:42[A]:LEU:HD11  | 1:N:4:PRO:HD2       | 2.02                     | 0.42              |
| 2:H:508:CMQ:C6      | 5:H:4086:HOH:O      | 2.67                     | 0.42              |
| 1:L:120[A]:MET:HE1  | 1:L:122:HIS:ND1     | 2.34                     | 0.42              |
| 1:N:94:GLN:HA       | 1:N:118:ARG:O       | 2.19                     | 0.42              |
| 1:E:17:PHE:HD2      | 1:E:21:SER:HB3      | 1.84                     | 0.42              |
| 1:B:189:LEU:HD22    | 1:B:193:ASN:HD21    | 1.84                     | 0.42              |
| 1:K:98:MET:HB2      | 1:K:98:MET:HE2      | 1.77                     | 0.42              |
| 2:K:511:CMQ:H22A    | 5:K:4029:HOH:O      | 2.19                     | 0.42              |
| 1:M:62:TYR:CD2      | 1:M:92[A]:MET:HE3   | 2.55                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:B:139:ALA:O      | 1:B:143:LEU:HG      | 2.19                     | 0.41              |
| 1:J:34:GLN:NE2     | 1:J:68:GLY:HA2      | 2.33                     | 0.41              |
| 1:J:176:ALA:HB3    | 1:J:177:PRO:HD3     | 2.02                     | 0.41              |
| 1:J:193:ASN:HD22   | 1:J:193:ASN:N       | 2.16                     | 0.41              |
| 1:L:3:VAL:HA       | 1:L:4:PRO:HD3       | 1.95                     | 0.41              |
| 1:C:122:HIS:CD2    | 2:C:503:CMQ:H242    | 2.34                     | 0.41              |
| 1:N:138:HIS:O      | 1:N:142[B]:ILE:HG13 | 2.21                     | 0.41              |
| 1:G:57:LYS:O       | 1:G:85:PRO:HB3      | 2.20                     | 0.41              |
| 1:H:22:ARG:O       | 1:H:25:LYS:HB2      | 2.21                     | 0.41              |
| 1:I:185[B]:VAL:CG2 | 1:I:186:ASP:N       | 2.84                     | 0.41              |
| 1:B:178:GLU:C      | 1:B:181:GLU:HG2     | 2.45                     | 0.41              |
| 1:H:145:VAL:O      | 1:H:149:MET:HG2     | 2.19                     | 0.41              |
| 1:K:7:ILE:HG12     | 1:K:8:GLU:H         | 1.86                     | 0.41              |
| 1:N:145:VAL:O      | 1:N:149:MET:HG2     | 2.20                     | 0.41              |
| 1:G:175:SER:OG     | 1:G:177:PRO:HD2     | 2.21                     | 0.41              |
| 1:J:92:MET:HB3     | 1:J:114:LEU:HD23    | 2.03                     | 0.41              |
| 1:K:175:SER:OG     | 1:K:177:PRO:HD2     | 2.20                     | 0.41              |
| 1:M:15:ARG:HG2     | 1:M:15:ARG:NH2      | 2.31                     | 0.41              |
| 1:B:115:PRO:HD3    | 1:B:189:LEU:O       | 2.20                     | 0.41              |
| 1:F:115:PRO:HG3    | 1:F:190:THR:HG22    | 2.02                     | 0.41              |
| 1:L:32:THR:OG1     | 1:M:41:ASN:ND2      | 2.53                     | 0.41              |
| 1:A:3:VAL:HG13     | 1:A:19:ILE:HG22     | 2.03                     | 0.41              |
| 1:A:62:TYR:CD2     | 1:A:92:MET:HE3      | 2.56                     | 0.41              |
| 1:A:108:LYS:HA     | 1:A:108:LYS:HD2     | 1.77                     | 0.41              |
| 1:B:38:HIS:HD2     | 5:B:4128:HOH:O      | 2.04                     | 0.41              |
| 1:D:92:MET:HB3     | 1:D:114:LEU:HD22    | 2.03                     | 0.41              |
| 1:E:135:ILE:HD13   | 1:L:142[A]:ILE:HD13 | 2.02                     | 0.41              |
| 1:J:8:GLU:CD       | 1:J:22:ARG:HE       | 2.29                     | 0.41              |
| 1:K:92:MET:HB3     | 1:K:114[A]:LEU:HD12 | 2.03                     | 0.41              |
| 1:L:16:SER:O       | 1:L:17:PHE:C        | 2.64                     | 0.41              |
| 1:A:2:LEU:HD13     | 1:G:3:VAL:HG21      | 2.02                     | 0.41              |
| 1:C:4:PRO:HG2      | 1:C:19:ILE:HB       | 2.03                     | 0.41              |
| 1:D:127:GLY:HA2    | 1:K:128:TYR:O       | 2.21                     | 0.41              |
| 1:H:189:LEU:HD23   | 1:H:189:LEU:HA      | 1.92                     | 0.41              |
| 1:K:70:ILE:O       | 1:K:74:MET:HG2      | 2.21                     | 0.41              |
| 1:L:136[B]:GLU:CD  | 1:L:140:ARG:HH11    | 2.28                     | 0.41              |
| 2:J:510:CMQ:H21A   | 5:J:4178:HOH:O      | 2.20                     | 0.40              |
| 1:M:34[A]:GLN:CG   | 5:M:4144:HOH:O      | 2.68                     | 0.40              |
| 1:N:41:ASN:ND2     | 5:N:4045:HOH:O      | 2.53                     | 0.40              |
| 2:B:502:CMQ:H22A   | 5:B:4038:HOH:O      | 2.21                     | 0.40              |
| 1:C:71:THR:HG21    | 4:C:3006:GOL:H2     | 2.03                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:73:GLY:HA3  | 1:H:98:MET:HE2  | 2.04                     | 0.40              |
| 1:I:54:ASN:ND2  | 1:I:57:LYS:HG3  | 2.37                     | 0.40              |
| 1:I:145:VAL:O   | 1:I:149:MET:HG2 | 2.22                     | 0.40              |
| 1:I:166:ARG:HG2 | 5:I:4080:HOH:O  | 2.20                     | 0.40              |
| 1:L:34:GLN:HE22 | 1:L:68:GLY:HA2  | 1.86                     | 0.40              |
| 1:H:139:ALA:O   | 1:H:143:LEU:HG  | 2.20                     | 0.40              |
| 1:K:21:SER:O    | 1:K:24:LEU:HB3  | 2.21                     | 0.40              |
| 1:M:57:LYS:O    | 1:M:85:PRO:HB3  | 2.21                     | 0.40              |
| 1:A:7:ILE:HB    | 1:G:17:PHE:CE2  | 2.57                     | 0.40              |
| 1:H:50:LEU:HD23 | 1:H:50:LEU:HA   | 1.86                     | 0.40              |
| 1:M:192:ARG:HG2 | 1:N:84:LYS:HE3  | 2.04                     | 0.40              |
| 1:G:115:PRO:HD3 | 1:G:189:LEU:O   | 2.21                     | 0.40              |
| 1:G:123:GLN:HB2 | 1:G:124:PRO:HD2 | 2.04                     | 0.40              |
| 1:H:2:LEU:HD13  | 5:I:4122:HOH:O  | 2.20                     | 0.40              |
| 1:I:84:LYS:NZ   | 5:I:4148:HOH:O  | 2.54                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 189/193 (98%)  | 184 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | B     | 200/193 (104%) | 195 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | C     | 186/193 (96%)  | 182 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | D     | 184/193 (95%)  | 180 (98%) | 3 (2%)  | 1 (0%)   | 24          | 16  |
| 1   | E     | 186/193 (96%)  | 180 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | F     | 183/193 (95%)  | 180 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | G     | 183/193 (95%)  | 179 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | H     | 181/193 (94%)  | 178 (98%) | 3 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | I     | 186/193 (96%)   | 183 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | J     | 183/193 (95%)   | 179 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | K     | 183/193 (95%)   | 178 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | L     | 190/193 (98%)   | 187 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | M     | 193/193 (100%)  | 188 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | N     | 189/193 (98%)   | 186 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| All | All   | 2616/2702 (97%) | 2559 (98%) | 56 (2%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 17  | PHE  |

### 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     | 165/163 (101%) | 151 (92%) | 14 (8%)  | 10          | 4  |
| 1   | B     | 173/163 (106%) | 160 (92%) | 13 (8%)  | 12          | 6  |
| 1   | C     | 162/163 (99%)  | 147 (91%) | 15 (9%)  | 8           | 3  |
| 1   | D     | 160/163 (98%)  | 149 (93%) | 11 (7%)  | 14          | 7  |
| 1   | E     | 161/163 (99%)  | 153 (95%) | 8 (5%)   | 22          | 14 |
| 1   | F     | 158/163 (97%)  | 148 (94%) | 10 (6%)  | 16          | 8  |
| 1   | G     | 159/163 (98%)  | 151 (95%) | 8 (5%)   | 22          | 14 |
| 1   | H     | 157/163 (96%)  | 146 (93%) | 11 (7%)  | 14          | 7  |
| 1   | I     | 162/163 (99%)  | 155 (96%) | 7 (4%)   | 26          | 18 |
| 1   | J     | 159/163 (98%)  | 149 (94%) | 10 (6%)  | 16          | 8  |
| 1   | K     | 159/163 (98%)  | 151 (95%) | 8 (5%)   | 22          | 14 |
| 1   | L     | 166/163 (102%) | 156 (94%) | 10 (6%)  | 17          | 9  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |
|-----|-------|------------------|------------|----------|-------------|
| 1   | M     | 168/163 (103%)   | 157 (94%)  | 11 (6%)  | 15 8        |
| 1   | N     | 165/163 (101%)   | 156 (94%)  | 9 (6%)   | 19 11       |
| All | All   | 2274/2282 (100%) | 2129 (94%) | 145 (6%) | 18 8        |

All (145) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 2      | LEU  |
| 1   | A     | 25     | LYS  |
| 1   | A     | 54     | ASN  |
| 1   | A     | 56     | GLU  |
| 1   | A     | 98[A]  | MET  |
| 1   | A     | 98[B]  | MET  |
| 1   | A     | 108    | LYS  |
| 1   | A     | 114    | LEU  |
| 1   | A     | 140    | ARG  |
| 1   | A     | 148    | ARG  |
| 1   | A     | 184[A] | LEU  |
| 1   | A     | 184[B] | LEU  |
| 1   | A     | 189[A] | LEU  |
| 1   | A     | 189[B] | LEU  |
| 1   | B     | 6      | VAL  |
| 1   | B     | 11     | SER  |
| 1   | B     | 31     | LEU  |
| 1   | B     | 36     | GLU  |
| 1   | B     | 108    | LYS  |
| 1   | B     | 114[A] | LEU  |
| 1   | B     | 114[B] | LEU  |
| 1   | B     | 148[A] | ARG  |
| 1   | B     | 148[B] | ARG  |
| 1   | B     | 162[A] | GLU  |
| 1   | B     | 162[B] | GLU  |
| 1   | B     | 184    | LEU  |
| 1   | B     | 193    | ASN  |
| 1   | C     | 5      | MET  |
| 1   | C     | 6      | VAL  |
| 1   | C     | 15     | ARG  |
| 1   | C     | 22     | ARG  |
| 1   | C     | 31     | LEU  |
| 1   | C     | 34     | GLN  |
| 1   | C     | 35     | VAL  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | C     | 36     | GLU  |
| 1   | C     | 42[A]  | LEU  |
| 1   | C     | 42[B]  | LEU  |
| 1   | C     | 84     | LYS  |
| 1   | C     | 114    | LEU  |
| 1   | C     | 143    | LEU  |
| 1   | C     | 148    | ARG  |
| 1   | C     | 185    | VAL  |
| 1   | D     | 2      | LEU  |
| 1   | D     | 3      | VAL  |
| 1   | D     | 8      | GLU  |
| 1   | D     | 17     | PHE  |
| 1   | D     | 22     | ARG  |
| 1   | D     | 26     | GLU  |
| 1   | D     | 31     | LEU  |
| 1   | D     | 129[A] | GLN  |
| 1   | D     | 129[B] | GLN  |
| 1   | D     | 136    | GLU  |
| 1   | D     | 185    | VAL  |
| 1   | E     | 6      | VAL  |
| 1   | E     | 8      | GLU  |
| 1   | E     | 19     | ILE  |
| 1   | E     | 26     | GLU  |
| 1   | E     | 31     | LEU  |
| 1   | E     | 36     | GLU  |
| 1   | E     | 148    | ARG  |
| 1   | E     | 184    | LEU  |
| 1   | F     | 3      | VAL  |
| 1   | F     | 6      | VAL  |
| 1   | F     | 18     | ASP  |
| 1   | F     | 21     | SER  |
| 1   | F     | 25     | LYS  |
| 1   | F     | 122    | HIS  |
| 1   | F     | 129    | GLN  |
| 1   | F     | 148    | ARG  |
| 1   | F     | 181    | GLU  |
| 1   | F     | 187    | SER  |
| 1   | G     | 6      | VAL  |
| 1   | G     | 22     | ARG  |
| 1   | G     | 36[A]  | GLU  |
| 1   | G     | 36[B]  | GLU  |
| 1   | G     | 54     | ASN  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | G     | 114    | LEU  |
| 1   | G     | 166    | ARG  |
| 1   | G     | 184    | LEU  |
| 1   | H     | 2      | LEU  |
| 1   | H     | 5      | MET  |
| 1   | H     | 16     | SER  |
| 1   | H     | 23     | LEU  |
| 1   | H     | 31     | LEU  |
| 1   | H     | 35     | VAL  |
| 1   | H     | 56     | GLU  |
| 1   | H     | 104    | THR  |
| 1   | H     | 120    | MET  |
| 1   | H     | 172    | ARG  |
| 1   | H     | 193    | ASN  |
| 1   | I     | 2      | LEU  |
| 1   | I     | 27     | ARG  |
| 1   | I     | 114    | LEU  |
| 1   | I     | 148    | ARG  |
| 1   | I     | 152[A] | LEU  |
| 1   | I     | 152[B] | LEU  |
| 1   | I     | 181    | GLU  |
| 1   | J     | 2      | LEU  |
| 1   | J     | 25     | LYS  |
| 1   | J     | 26     | GLU  |
| 1   | J     | 31     | LEU  |
| 1   | J     | 56     | GLU  |
| 1   | J     | 80[A]  | MET  |
| 1   | J     | 80[B]  | MET  |
| 1   | J     | 114    | LEU  |
| 1   | J     | 122    | HIS  |
| 1   | J     | 193    | ASN  |
| 1   | K     | 2      | LEU  |
| 1   | K     | 6      | VAL  |
| 1   | K     | 16     | SER  |
| 1   | K     | 18     | ASP  |
| 1   | K     | 42     | LEU  |
| 1   | K     | 148    | ARG  |
| 1   | K     | 153    | MET  |
| 1   | K     | 172    | ARG  |
| 1   | L     | 3      | VAL  |
| 1   | L     | 25     | LYS  |
| 1   | L     | 56     | GLU  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | L     | 104[A] | THR  |
| 1   | L     | 104[B] | THR  |
| 1   | L     | 114    | LEU  |
| 1   | L     | 148    | ARG  |
| 1   | L     | 181[A] | GLU  |
| 1   | L     | 181[B] | GLU  |
| 1   | L     | 193    | ASN  |
| 1   | M     | 16     | SER  |
| 1   | M     | 22     | ARG  |
| 1   | M     | 31[A]  | LEU  |
| 1   | M     | 31[B]  | LEU  |
| 1   | M     | 56     | GLU  |
| 1   | M     | 108[A] | LYS  |
| 1   | M     | 108[B] | LYS  |
| 1   | M     | 114    | LEU  |
| 1   | M     | 153    | MET  |
| 1   | M     | 163    | GLN  |
| 1   | M     | 192    | ARG  |
| 1   | N     | 3      | VAL  |
| 1   | N     | 18     | ASP  |
| 1   | N     | 31[A]  | LEU  |
| 1   | N     | 31[B]  | LEU  |
| 1   | N     | 36[A]  | GLU  |
| 1   | N     | 36[B]  | GLU  |
| 1   | N     | 114[A] | LEU  |
| 1   | N     | 114[B] | LEU  |
| 1   | N     | 148    | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 41  | ASN  |
| 1   | A     | 54  | ASN  |
| 1   | A     | 123 | GLN  |
| 1   | A     | 156 | HIS  |
| 1   | A     | 163 | GLN  |
| 1   | B     | 34  | GLN  |
| 1   | B     | 38  | HIS  |
| 1   | B     | 41  | ASN  |
| 1   | B     | 116 | ASN  |
| 1   | B     | 123 | GLN  |
| 1   | B     | 163 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 193 | ASN  |
| 1   | C     | 41  | ASN  |
| 1   | C     | 116 | ASN  |
| 1   | D     | 34  | GLN  |
| 1   | D     | 41  | ASN  |
| 1   | D     | 156 | HIS  |
| 1   | D     | 193 | ASN  |
| 1   | E     | 34  | GLN  |
| 1   | E     | 38  | HIS  |
| 1   | E     | 41  | ASN  |
| 1   | E     | 116 | ASN  |
| 1   | E     | 123 | GLN  |
| 1   | E     | 129 | GLN  |
| 1   | E     | 156 | HIS  |
| 1   | F     | 38  | HIS  |
| 1   | F     | 41  | ASN  |
| 1   | F     | 123 | GLN  |
| 1   | F     | 163 | GLN  |
| 1   | F     | 191 | HIS  |
| 1   | G     | 41  | ASN  |
| 1   | G     | 54  | ASN  |
| 1   | G     | 191 | HIS  |
| 1   | H     | 34  | GLN  |
| 1   | H     | 41  | ASN  |
| 1   | H     | 159 | GLN  |
| 1   | H     | 193 | ASN  |
| 1   | I     | 34  | GLN  |
| 1   | I     | 41  | ASN  |
| 1   | J     | 41  | ASN  |
| 1   | J     | 116 | ASN  |
| 1   | J     | 123 | GLN  |
| 1   | J     | 193 | ASN  |
| 1   | K     | 34  | GLN  |
| 1   | K     | 41  | ASN  |
| 1   | K     | 123 | GLN  |
| 1   | K     | 191 | HIS  |
| 1   | K     | 193 | ASN  |
| 1   | L     | 123 | GLN  |
| 1   | L     | 193 | ASN  |
| 1   | M     | 41  | ASN  |
| 1   | M     | 116 | ASN  |
| 1   | M     | 123 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 163 | GLN  |
| 1   | N     | 34  | GLN  |
| 1   | N     | 41  | ASN  |
| 1   | N     | 94  | GLN  |
| 1   | N     | 123 | GLN  |
| 1   | N     | 163 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

40 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | CMQ  | H     | 508  | 1    | 31,32,32     | 1.21 | 1 (3%)   | 40,42,42    | 1.71 | 9 (22%)  |
| 3   | PGE  | D     | 4004 | -    | 9,9,9        | 0.48 | 0        | 8,8,8       | 0.34 | 0        |
| 3   | PGE  | K     | 4011 | -    | 9,9,9        | 0.52 | 0        | 8,8,8       | 0.45 | 0        |
| 3   | PGE  | B     | 4002 | -    | 9,9,9        | 0.51 | 0        | 8,8,8       | 0.18 | 0        |
| 3   | PGE  | A     | 4001 | -    | 9,9,9        | 0.51 | 0        | 8,8,8       | 0.29 | 0        |
| 4   | GOL  | G     | 3009 | -    | 5,5,5        | 0.51 | 0        | 5,5,5       | 0.38 | 0        |
| 2   | CMQ  | G     | 507  | 1    | 31,32,32     | 1.43 | 3 (9%)   | 40,42,42    | 1.40 | 7 (17%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | GOL  | N     | 3007 | -    | 5,5,5        | 0.31 | 0        | 5,5,5       | 0.79 | 0        |
| 4   | GOL  | A     | 3001 | -    | 5,5,5        | 0.30 | 0        | 5,5,5       | 0.52 | 0        |
| 4   | GOL  | H     | 3008 | -    | 5,5,5        | 0.38 | 0        | 5,5,5       | 0.95 | 0        |
| 3   | PGE  | F     | 4006 | -    | 9,9,9        | 0.38 | 0        | 8,8,8       | 0.51 | 0        |
| 2   | CMQ  | J     | 510  | 1    | 31,32,32     | 1.22 | 1 (3%)   | 40,42,42    | 1.59 | 7 (17%)  |
| 2   | CMQ  | B     | 502  | 1    | 31,32,32     | 1.12 | 1 (3%)   | 40,42,42    | 1.51 | 4 (10%)  |
| 2   | CMQ  | C     | 503  | 1    | 31,32,32     | 1.25 | 2 (6%)   | 40,42,42    | 1.48 | 6 (15%)  |
| 3   | PGE  | G     | 4007 | -    | 9,9,9        | 0.50 | 0        | 8,8,8       | 0.48 | 0        |
| 2   | CMQ  | A     | 501  | 1    | 31,32,32     | 1.26 | 2 (6%)   | 40,42,42    | 1.69 | 9 (22%)  |
| 3   | PGE  | L     | 4012 | -    | 9,9,9        | 0.59 | 0        | 8,8,8       | 0.31 | 0        |
| 4   | GOL  | B     | 3003 | -    | 5,5,5        | 0.44 | 0        | 5,5,5       | 0.37 | 0        |
| 2   | CMQ  | E     | 505  | 1    | 31,32,32     | 1.34 | 2 (6%)   | 40,42,42    | 1.82 | 12 (30%) |
| 2   | CMQ  | N     | 514  | 1    | 31,32,32     | 1.24 | 1 (3%)   | 40,42,42    | 1.19 | 4 (10%)  |
| 2   | CMQ  | M     | 513  | 1    | 31,32,32     | 1.20 | 2 (6%)   | 40,42,42    | 1.33 | 3 (7%)   |
| 2   | CMQ  | D     | 504  | 1    | 31,32,32     | 1.21 | 1 (3%)   | 40,42,42    | 1.57 | 7 (17%)  |
| 2   | CMQ  | L     | 512  | 1    | 31,32,32     | 1.24 | 2 (6%)   | 40,42,42    | 1.43 | 6 (15%)  |
| 4   | GOL  | K     | 3010 | -    | 5,5,5        | 0.34 | 0        | 5,5,5       | 0.86 | 0        |
| 4   | GOL  | C     | 3006 | -    | 5,5,5        | 0.35 | 0        | 5,5,5       | 0.59 | 0        |
| 3   | PGE  | J     | 4010 | -    | 9,9,9        | 0.61 | 0        | 8,8,8       | 0.48 | 0        |
| 4   | GOL  | F     | 3004 | -    | 5,5,5        | 0.61 | 0        | 5,5,5       | 0.76 | 0        |
| 4   | GOL  | B     | 3002 | -    | 5,5,5        | 0.23 | 0        | 5,5,5       | 0.67 | 0        |
| 3   | PGE  | I     | 4009 | -    | 9,9,9        | 0.45 | 0        | 8,8,8       | 0.45 | 0        |
| 3   | PGE  | E     | 4005 | -    | 9,9,9        | 0.49 | 0        | 8,8,8       | 0.36 | 0        |
| 2   | CMQ  | F     | 506  | 1    | 31,32,32     | 1.16 | 1 (3%)   | 40,42,42    | 1.43 | 7 (17%)  |
| 3   | PGE  | C     | 4003 | -    | 9,9,9        | 0.51 | 0        | 8,8,8       | 0.31 | 0        |
| 3   | PGE  | N     | 4014 | -    | 9,9,9        | 0.44 | 0        | 8,8,8       | 0.45 | 0        |
| 4   | GOL  | C     | 3005 | -    | 5,5,5        | 0.28 | 0        | 5,5,5       | 0.67 | 0        |
| 3   | PGE  | H     | 4008 | -    | 9,9,9        | 0.43 | 0        | 8,8,8       | 0.53 | 0        |
| 2   | CMQ  | K     | 511  | 1    | 31,32,32     | 1.15 | 1 (3%)   | 40,42,42    | 1.34 | 6 (15%)  |
| 3   | PGE  | K     | 4015 | -    | 9,9,9        | 0.23 | 0        | 8,8,8       | 0.89 | 0        |
| 4   | GOL  | L     | 3011 | -    | 5,5,5        | 0.46 | 0        | 5,5,5       | 0.69 | 0        |
| 3   | PGE  | M     | 4013 | -    | 9,9,9        | 0.43 | 0        | 8,8,8       | 0.50 | 0        |
| 2   | CMQ  | I     | 509  | 1    | 31,32,32     | 1.21 | 1 (3%)   | 40,42,42    | 1.79 | 9 (22%)  |

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   | CMQ  | H     | 508  | 1    | -       | 9/29/29/29  | 0/2/2/2 |
| 3   | PGE  | D     | 4004 | -    | -       | 5/7/7/7     | -       |
| 3   | PGE  | K     | 4011 | -    | -       | 5/7/7/7     | -       |
| 3   | PGE  | B     | 4002 | -    | -       | 3/7/7/7     | -       |
| 3   | PGE  | A     | 4001 | -    | -       | 3/7/7/7     | -       |
| 4   | GOL  | G     | 3009 | -    | -       | 2/4/4/4     | -       |
| 2   | CMQ  | G     | 507  | 1    | -       | 5/29/29/29  | 0/2/2/2 |
| 4   | GOL  | N     | 3007 | -    | -       | 4/4/4/4     | -       |
| 4   | GOL  | A     | 3001 | -    | -       | 2/4/4/4     | -       |
| 4   | GOL  | H     | 3008 | -    | -       | 0/4/4/4     | -       |
| 3   | PGE  | F     | 4006 | -    | -       | 6/7/7/7     | -       |
| 2   | CMQ  | J     | 510  | 1    | -       | 9/29/29/29  | 0/2/2/2 |
| 2   | CMQ  | B     | 502  | 1    | -       | 6/29/29/29  | 0/2/2/2 |
| 2   | CMQ  | C     | 503  | 1    | -       | 6/29/29/29  | 0/2/2/2 |
| 3   | PGE  | G     | 4007 | -    | -       | 5/7/7/7     | -       |
| 2   | CMQ  | A     | 501  | 1    | -       | 4/29/29/29  | 0/2/2/2 |
| 3   | PGE  | L     | 4012 | -    | -       | 4/7/7/7     | -       |
| 4   | GOL  | B     | 3003 | -    | -       | 2/4/4/4     | -       |
| 2   | CMQ  | E     | 505  | 1    | -       | 10/29/29/29 | 0/2/2/2 |
| 2   | CMQ  | N     | 514  | 1    | -       | 9/29/29/29  | 0/2/2/2 |
| 2   | CMQ  | M     | 513  | 1    | -       | 7/29/29/29  | 0/2/2/2 |
| 2   | CMQ  | D     | 504  | 1    | -       | 8/29/29/29  | 0/2/2/2 |
| 2   | CMQ  | L     | 512  | 1    | -       | 8/29/29/29  | 0/2/2/2 |
| 4   | GOL  | K     | 3010 | -    | -       | 3/4/4/4     | -       |
| 4   | GOL  | C     | 3006 | -    | -       | 2/4/4/4     | -       |
| 3   | PGE  | J     | 4010 | -    | -       | 0/7/7/7     | -       |
| 4   | GOL  | F     | 3004 | -    | -       | 2/4/4/4     | -       |
| 4   | GOL  | B     | 3002 | -    | -       | 1/4/4/4     | -       |
| 3   | PGE  | I     | 4009 | -    | -       | 3/7/7/7     | -       |
| 3   | PGE  | E     | 4005 | -    | -       | 4/7/7/7     | -       |
| 2   | CMQ  | F     | 506  | 1    | -       | 4/29/29/29  | 0/2/2/2 |
| 3   | PGE  | C     | 4003 | -    | -       | 6/7/7/7     | -       |
| 3   | PGE  | N     | 4014 | -    | -       | 3/7/7/7     | -       |
| 4   | GOL  | C     | 3005 | -    | -       | 4/4/4/4     | -       |
| 3   | PGE  | H     | 4008 | -    | -       | 3/7/7/7     | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | CMQ  | K     | 511  | 1    | -       | 7/29/29/29 | 0/2/2/2 |
| 3   | PGE  | K     | 4015 | -    | -       | 6/7/7/7    | -       |
| 4   | GOL  | L     | 3011 | -    | -       | 2/4/4/4    | -       |
| 3   | PGE  | M     | 4013 | -    | -       | 3/7/7/7    | -       |
| 2   | CMQ  | I     | 509  | 1    | -       | 5/29/29/29 | 0/2/2/2 |

All (21) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | G     | 507 | CMQ  | O1-C1   | 5.95 | 1.47        | 1.35     |
| 2   | C     | 503 | CMQ  | O1-C1   | 5.70 | 1.46        | 1.35     |
| 2   | D     | 504 | CMQ  | O1-C1   | 5.57 | 1.46        | 1.35     |
| 2   | J     | 510 | CMQ  | O1-C1   | 5.34 | 1.45        | 1.35     |
| 2   | H     | 508 | CMQ  | O1-C1   | 5.18 | 1.45        | 1.35     |
| 2   | A     | 501 | CMQ  | O1-C1   | 5.15 | 1.45        | 1.35     |
| 2   | E     | 505 | CMQ  | O1-C1   | 5.11 | 1.45        | 1.35     |
| 2   | K     | 511 | CMQ  | O1-C1   | 4.91 | 1.45        | 1.35     |
| 2   | L     | 512 | CMQ  | O1-C1   | 4.87 | 1.44        | 1.35     |
| 2   | I     | 509 | CMQ  | O1-C1   | 4.84 | 1.44        | 1.35     |
| 2   | N     | 514 | CMQ  | O1-C1   | 4.68 | 1.44        | 1.35     |
| 2   | B     | 502 | CMQ  | O1-C1   | 4.65 | 1.44        | 1.35     |
| 2   | F     | 506 | CMQ  | O1-C1   | 4.38 | 1.44        | 1.35     |
| 2   | M     | 513 | CMQ  | O1-C1   | 3.87 | 1.42        | 1.35     |
| 2   | M     | 513 | CMQ  | O2-C1   | 2.57 | 1.26        | 1.21     |
| 2   | C     | 503 | CMQ  | C21-C19 | 2.33 | 1.42        | 1.38     |
| 2   | L     | 512 | CMQ  | C20-C22 | 2.23 | 1.42        | 1.38     |
| 2   | A     | 501 | CMQ  | C20-C22 | 2.13 | 1.42        | 1.38     |
| 2   | G     | 507 | CMQ  | C21-C19 | 2.13 | 1.42        | 1.38     |
| 2   | E     | 505 | CMQ  | C21-C19 | 2.04 | 1.42        | 1.38     |
| 2   | G     | 507 | CMQ  | C24-C16 | 2.04 | 1.57        | 1.51     |

All (96) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | E     | 505 | CMQ  | C16-C15-N2 | -5.67 | 100.61      | 110.90   |
| 2   | I     | 509 | CMQ  | O1-C1-O2   | -5.43 | 113.85      | 124.26   |
| 2   | A     | 501 | CMQ  | C16-C15-N2 | -5.39 | 101.12      | 110.90   |
| 2   | B     | 502 | CMQ  | C16-C15-N2 | -5.36 | 101.17      | 110.90   |
| 2   | I     | 509 | CMQ  | C16-C15-N2 | -5.34 | 101.20      | 110.90   |
| 2   | H     | 508 | CMQ  | C16-C15-N2 | -4.87 | 102.06      | 110.90   |
| 2   | J     | 510 | CMQ  | C16-C15-N2 | -4.41 | 102.90      | 110.90   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | E     | 505 | CMQ  | O1-C1-O2    | -4.34 | 115.95      | 124.26   |
| 2   | D     | 504 | CMQ  | O1-C1-N1    | 4.29  | 119.62      | 110.45   |
| 2   | B     | 502 | CMQ  | O1-C1-N1    | 4.28  | 119.60      | 110.45   |
| 2   | C     | 503 | CMQ  | C17-C15-N2  | -4.18 | 104.14      | 110.08   |
| 2   | B     | 502 | CMQ  | O1-C1-O2    | -4.09 | 116.42      | 124.26   |
| 2   | F     | 506 | CMQ  | C17-C15-N2  | -4.06 | 104.31      | 110.08   |
| 2   | D     | 504 | CMQ  | O1-C1-O2    | -3.98 | 116.62      | 124.26   |
| 2   | M     | 513 | CMQ  | C17-C15-N2  | -3.97 | 104.44      | 110.08   |
| 2   | C     | 503 | CMQ  | C16-C15-N2  | -3.93 | 103.76      | 110.90   |
| 2   | K     | 511 | CMQ  | C16-C15-N2  | -3.91 | 103.80      | 110.90   |
| 2   | L     | 512 | CMQ  | C16-C15-N2  | -3.85 | 103.91      | 110.90   |
| 2   | L     | 512 | CMQ  | O1-C1-O2    | -3.79 | 117.00      | 124.26   |
| 2   | L     | 512 | CMQ  | O1-C1-N1    | 3.78  | 118.53      | 110.45   |
| 2   | J     | 510 | CMQ  | C17-C15-N2  | -3.73 | 104.78      | 110.08   |
| 2   | G     | 507 | CMQ  | C16-C15-N2  | -3.68 | 104.22      | 110.90   |
| 2   | M     | 513 | CMQ  | O1-C1-O2    | -3.67 | 117.23      | 124.26   |
| 2   | C     | 503 | CMQ  | O1-C1-O2    | -3.66 | 117.23      | 124.26   |
| 2   | A     | 501 | CMQ  | O1-C1-O2    | -3.66 | 117.24      | 124.26   |
| 2   | H     | 508 | CMQ  | C11-C9-N1   | -3.59 | 102.47      | 110.58   |
| 2   | H     | 508 | CMQ  | C17-C15-N2  | -3.43 | 105.21      | 110.08   |
| 2   | I     | 509 | CMQ  | O1-C1-N1    | 3.41  | 117.73      | 110.45   |
| 2   | K     | 511 | CMQ  | O1-C1-O2    | -3.40 | 117.74      | 124.26   |
| 2   | J     | 510 | CMQ  | C9-N1-C1    | 3.35  | 129.26      | 120.93   |
| 2   | C     | 503 | CMQ  | O1-C1-N1    | 3.35  | 117.61      | 110.45   |
| 2   | L     | 512 | CMQ  | C17-C15-N2  | -3.34 | 105.34      | 110.08   |
| 2   | A     | 501 | CMQ  | C17-C15-N2  | -3.31 | 105.39      | 110.08   |
| 2   | J     | 510 | CMQ  | C10-C9-N1   | -3.29 | 102.21      | 111.11   |
| 2   | F     | 506 | CMQ  | C16-C15-N2  | -3.22 | 105.06      | 110.90   |
| 2   | D     | 504 | CMQ  | C17-C15-N2  | -3.15 | 105.61      | 110.08   |
| 2   | J     | 510 | CMQ  | O4-C16-C24  | -3.13 | 100.32      | 109.68   |
| 2   | H     | 508 | CMQ  | O1-C1-O2    | -3.05 | 118.42      | 124.26   |
| 2   | G     | 507 | CMQ  | O1-C1-O2    | -3.03 | 118.45      | 124.26   |
| 2   | M     | 513 | CMQ  | O1-C2-C3    | 2.95  | 116.57      | 109.40   |
| 2   | D     | 504 | CMQ  | C13-C12-C11 | 2.94  | 121.66      | 111.08   |
| 2   | E     | 505 | CMQ  | O1-C1-N1    | 2.93  | 116.72      | 110.45   |
| 2   | H     | 508 | CMQ  | O1-C2-C3    | 2.92  | 116.48      | 109.40   |
| 2   | N     | 514 | CMQ  | C17-C15-N2  | -2.91 | 105.95      | 110.08   |
| 2   | F     | 506 | CMQ  | O1-C1-O2    | -2.89 | 118.71      | 124.26   |
| 2   | K     | 511 | CMQ  | O1-C1-N1    | 2.86  | 116.57      | 110.45   |
| 2   | B     | 502 | CMQ  | O1-C2-C3    | 2.86  | 116.34      | 109.40   |
| 2   | N     | 514 | CMQ  | O1-C1-O2    | -2.84 | 118.81      | 124.26   |
| 2   | E     | 505 | CMQ  | C11-C9-N1   | -2.82 | 104.22      | 110.58   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | J     | 510 | CMQ  | C11-C9-N1   | -2.82 | 104.22      | 110.58   |
| 2   | G     | 507 | CMQ  | C17-C15-N2  | -2.73 | 106.21      | 110.08   |
| 2   | I     | 509 | CMQ  | C9-N1-C1    | 2.73  | 127.72      | 120.93   |
| 2   | G     | 507 | CMQ  | C17-C15-C16 | 2.72  | 116.03      | 111.70   |
| 2   | E     | 505 | CMQ  | O4-C16-C24  | -2.71 | 101.57      | 109.68   |
| 2   | A     | 501 | CMQ  | C2-O1-C1    | -2.68 | 109.90      | 115.93   |
| 2   | A     | 501 | CMQ  | C8-C3-C4    | 2.67  | 122.20      | 118.23   |
| 2   | H     | 508 | CMQ  | C10-C9-N1   | -2.67 | 103.89      | 111.11   |
| 2   | L     | 512 | CMQ  | O1-C2-C3    | 2.66  | 115.87      | 109.40   |
| 2   | D     | 504 | CMQ  | C16-C15-N2  | -2.61 | 106.16      | 110.90   |
| 2   | H     | 508 | CMQ  | O4-C16-C24  | -2.57 | 101.98      | 109.68   |
| 2   | E     | 505 | CMQ  | C11-C9-C10  | -2.57 | 104.50      | 110.59   |
| 2   | F     | 506 | CMQ  | O1-C2-C3    | 2.56  | 115.62      | 109.40   |
| 2   | G     | 507 | CMQ  | O1-C2-C3    | 2.54  | 115.57      | 109.40   |
| 2   | F     | 506 | CMQ  | C10-C9-N1   | -2.51 | 104.32      | 111.11   |
| 2   | N     | 514 | CMQ  | C11-C9-C10  | -2.49 | 104.67      | 110.59   |
| 2   | C     | 503 | CMQ  | O1-C2-C3    | 2.49  | 115.45      | 109.40   |
| 2   | N     | 514 | CMQ  | C16-C15-N2  | -2.49 | 106.38      | 110.90   |
| 2   | H     | 508 | CMQ  | C12-C11-C9  | 2.49  | 122.09      | 115.40   |
| 2   | A     | 501 | CMQ  | C17-C15-C16 | 2.46  | 115.62      | 111.70   |
| 2   | F     | 506 | CMQ  | O1-C1-N1    | 2.45  | 115.70      | 110.45   |
| 2   | A     | 501 | CMQ  | C9-N1-C1    | 2.35  | 126.78      | 120.93   |
| 2   | K     | 511 | CMQ  | O4-C16-C24  | -2.33 | 102.70      | 109.68   |
| 2   | E     | 505 | CMQ  | O1-C2-C3    | 2.32  | 115.03      | 109.40   |
| 2   | E     | 505 | CMQ  | C17-C15-N2  | -2.32 | 106.79      | 110.08   |
| 2   | G     | 507 | CMQ  | C8-C3-C4    | 2.30  | 121.65      | 118.23   |
| 2   | D     | 504 | CMQ  | O1-C2-C3    | 2.29  | 114.96      | 109.40   |
| 2   | F     | 506 | CMQ  | C17-C15-C16 | 2.29  | 115.35      | 111.70   |
| 2   | K     | 511 | CMQ  | C17-C15-N2  | -2.28 | 106.85      | 110.08   |
| 2   | A     | 501 | CMQ  | C7-C8-C3    | -2.27 | 117.42      | 120.61   |
| 2   | E     | 505 | CMQ  | C18-C17-C15 | -2.23 | 109.61      | 113.40   |
| 2   | I     | 509 | CMQ  | C8-C3-C4    | 2.23  | 121.55      | 118.23   |
| 2   | J     | 510 | CMQ  | C11-C9-C10  | -2.23 | 105.30      | 110.59   |
| 2   | E     | 505 | CMQ  | C22-C20-C18 | -2.23 | 118.07      | 121.00   |
| 2   | E     | 505 | CMQ  | C8-C3-C4    | 2.22  | 121.54      | 118.23   |
| 2   | L     | 512 | CMQ  | C11-C9-C10  | -2.22 | 105.33      | 110.59   |
| 2   | E     | 505 | CMQ  | C2-O1-C1    | -2.20 | 110.97      | 115.93   |
| 2   | D     | 504 | CMQ  | C12-C11-C9  | 2.18  | 121.24      | 115.40   |
| 2   | H     | 508 | CMQ  | O1-C1-N1    | 2.17  | 115.09      | 110.45   |
| 2   | G     | 507 | CMQ  | O1-C1-N1    | 2.17  | 115.09      | 110.45   |
| 2   | I     | 509 | CMQ  | O2-C1-N1    | 2.17  | 128.41      | 124.86   |
| 2   | C     | 503 | CMQ  | O4-C16-C24  | -2.13 | 103.31      | 109.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 501 | CMQ  | O1-C1-N1    | 2.09  | 114.92      | 110.45   |
| 2   | I     | 509 | CMQ  | C17-C15-C16 | 2.08  | 115.02      | 111.70   |
| 2   | I     | 509 | CMQ  | C20-C22-C23 | 2.07  | 122.07      | 119.88   |
| 2   | K     | 511 | CMQ  | C10-C9-N1   | -2.04 | 105.60      | 111.11   |
| 2   | I     | 509 | CMQ  | C5-C4-C3    | -2.03 | 117.75      | 120.61   |

There are no chirality outliers.

All (180) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | A     | 501  | CMQ  | N2-C15-C17-C18  |
| 2   | A     | 501  | CMQ  | C16-C15-C17-C18 |
| 2   | B     | 502  | CMQ  | N2-C15-C17-C18  |
| 2   | B     | 502  | CMQ  | C16-C15-C17-C18 |
| 2   | C     | 503  | CMQ  | N2-C15-C17-C18  |
| 2   | C     | 503  | CMQ  | C16-C15-C17-C18 |
| 2   | D     | 504  | CMQ  | N2-C15-C17-C18  |
| 2   | D     | 504  | CMQ  | C16-C15-C17-C18 |
| 2   | E     | 505  | CMQ  | N2-C15-C17-C18  |
| 2   | E     | 505  | CMQ  | C16-C15-C17-C18 |
| 2   | F     | 506  | CMQ  | N2-C15-C17-C18  |
| 2   | F     | 506  | CMQ  | C16-C15-C17-C18 |
| 2   | G     | 507  | CMQ  | N2-C15-C17-C18  |
| 2   | G     | 507  | CMQ  | C16-C15-C17-C18 |
| 2   | H     | 508  | CMQ  | N2-C15-C17-C18  |
| 2   | H     | 508  | CMQ  | C16-C15-C17-C18 |
| 2   | I     | 509  | CMQ  | N2-C15-C17-C18  |
| 2   | I     | 509  | CMQ  | C16-C15-C17-C18 |
| 2   | J     | 510  | CMQ  | N2-C15-C17-C18  |
| 2   | J     | 510  | CMQ  | C16-C15-C17-C18 |
| 2   | K     | 511  | CMQ  | N2-C15-C17-C18  |
| 2   | K     | 511  | CMQ  | C16-C15-C17-C18 |
| 2   | L     | 512  | CMQ  | N2-C15-C17-C18  |
| 2   | L     | 512  | CMQ  | C16-C15-C17-C18 |
| 2   | M     | 513  | CMQ  | N2-C15-C17-C18  |
| 2   | M     | 513  | CMQ  | C16-C15-C17-C18 |
| 2   | N     | 514  | CMQ  | O2-C1-O1-C2     |
| 2   | N     | 514  | CMQ  | N1-C1-O1-C2     |
| 2   | N     | 514  | CMQ  | N2-C15-C17-C18  |
| 2   | N     | 514  | CMQ  | C16-C15-C17-C18 |
| 4   | A     | 3001 | GOL  | C1-C2-C3-O3     |
| 4   | B     | 3003 | GOL  | C1-C2-C3-O3     |

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| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 4   | C     | 3005 | GOL  | O1-C1-C2-C3    |
| 4   | C     | 3005 | GOL  | C1-C2-C3-O3    |
| 4   | F     | 3004 | GOL  | C1-C2-C3-O3    |
| 4   | K     | 3010 | GOL  | O1-C1-C2-C3    |
| 4   | L     | 3011 | GOL  | O1-C1-C2-O2    |
| 4   | L     | 3011 | GOL  | O1-C1-C2-C3    |
| 4   | N     | 3007 | GOL  | C1-C2-C3-O3    |
| 2   | A     | 501  | CMQ  | O2-C1-O1-C2    |
| 2   | C     | 503  | CMQ  | O2-C1-O1-C2    |
| 2   | D     | 504  | CMQ  | O2-C1-O1-C2    |
| 2   | E     | 505  | CMQ  | O2-C1-O1-C2    |
| 2   | H     | 508  | CMQ  | O2-C1-O1-C2    |
| 2   | L     | 512  | CMQ  | O2-C1-O1-C2    |
| 2   | D     | 504  | CMQ  | N1-C1-O1-C2    |
| 2   | E     | 505  | CMQ  | N1-C1-O1-C2    |
| 2   | I     | 509  | CMQ  | O2-C1-O1-C2    |
| 2   | J     | 510  | CMQ  | O2-C1-O1-C2    |
| 2   | M     | 513  | CMQ  | O2-C1-O1-C2    |
| 2   | A     | 501  | CMQ  | N1-C1-O1-C2    |
| 2   | C     | 503  | CMQ  | N1-C1-O1-C2    |
| 2   | H     | 508  | CMQ  | N1-C1-O1-C2    |
| 2   | J     | 510  | CMQ  | N1-C1-O1-C2    |
| 2   | L     | 512  | CMQ  | N1-C1-O1-C2    |
| 2   | M     | 513  | CMQ  | N1-C1-O1-C2    |
| 2   | B     | 502  | CMQ  | N1-C1-O1-C2    |
| 2   | I     | 509  | CMQ  | N1-C1-O1-C2    |
| 2   | B     | 502  | CMQ  | O2-C1-O1-C2    |
| 3   | C     | 4003 | PGE  | C6-C5-O3-C4    |
| 3   | C     | 4003 | PGE  | O2-C3-C4-O3    |
| 3   | G     | 4007 | PGE  | O2-C3-C4-O3    |
| 3   | K     | 4015 | PGE  | O2-C3-C4-O3    |
| 2   | J     | 510  | CMQ  | C12-C11-C9-N1  |
| 3   | K     | 4015 | PGE  | O3-C5-C6-O4    |
| 3   | L     | 4012 | PGE  | O3-C5-C6-O4    |
| 3   | E     | 4005 | PGE  | O2-C3-C4-O3    |
| 3   | G     | 4007 | PGE  | O1-C1-C2-O2    |
| 2   | D     | 504  | CMQ  | C9-C11-C12-C13 |
| 2   | E     | 505  | CMQ  | C9-C11-C12-C13 |
| 3   | K     | 4011 | PGE  | O2-C3-C4-O3    |
| 2   | H     | 508  | CMQ  | C9-C11-C12-C13 |
| 2   | H     | 508  | CMQ  | C12-C11-C9-N1  |
| 3   | A     | 4001 | PGE  | O1-C1-C2-O2    |

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| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 3   | B     | 4002 | PGE  | O1-C1-C2-O2    |
| 3   | C     | 4003 | PGE  | O3-C5-C6-O4    |
| 3   | G     | 4007 | PGE  | O3-C5-C6-O4    |
| 3   | H     | 4008 | PGE  | O1-C1-C2-O2    |
| 3   | M     | 4013 | PGE  | O3-C5-C6-O4    |
| 2   | K     | 511  | CMQ  | N1-C1-O1-C2    |
| 3   | G     | 4007 | PGE  | C6-C5-O3-C4    |
| 2   | J     | 510  | CMQ  | C9-C11-C12-C13 |
| 2   | K     | 511  | CMQ  | O2-C1-O1-C2    |
| 2   | N     | 514  | CMQ  | N2-C15-C16-O4  |
| 4   | C     | 3006 | GOL  | C1-C2-C3-O3    |
| 4   | G     | 3009 | GOL  | O1-C1-C2-C3    |
| 4   | N     | 3007 | GOL  | O1-C1-C2-C3    |
| 3   | D     | 4004 | PGE  | O1-C1-C2-O2    |
| 3   | F     | 4006 | PGE  | O3-C5-C6-O4    |
| 3   | I     | 4009 | PGE  | O3-C5-C6-O4    |
| 3   | K     | 4011 | PGE  | O1-C1-C2-O2    |
| 3   | B     | 4002 | PGE  | O2-C3-C4-O3    |
| 4   | B     | 3003 | GOL  | O2-C2-C3-O3    |
| 4   | C     | 3005 | GOL  | O1-C1-C2-O2    |
| 4   | C     | 3005 | GOL  | O2-C2-C3-O3    |
| 4   | C     | 3006 | GOL  | O2-C2-C3-O3    |
| 4   | F     | 3004 | GOL  | O2-C2-C3-O3    |
| 4   | G     | 3009 | GOL  | O1-C1-C2-O2    |
| 4   | K     | 3010 | GOL  | O1-C1-C2-O2    |
| 4   | N     | 3007 | GOL  | O2-C2-C3-O3    |
| 3   | D     | 4004 | PGE  | O3-C5-C6-O4    |
| 3   | E     | 4005 | PGE  | O3-C5-C6-O4    |
| 3   | K     | 4011 | PGE  | O3-C5-C6-O4    |
| 3   | F     | 4006 | PGE  | O1-C1-C2-O2    |
| 2   | D     | 504  | CMQ  | C9-C11-C12-C14 |
| 3   | N     | 4014 | PGE  | O2-C3-C4-O3    |
| 2   | D     | 504  | CMQ  | C12-C11-C9-N1  |
| 3   | E     | 4005 | PGE  | O1-C1-C2-O2    |
| 3   | K     | 4015 | PGE  | O1-C1-C2-O2    |
| 2   | N     | 514  | CMQ  | N2-C15-C16-C24 |
| 4   | N     | 3007 | GOL  | O1-C1-C2-O2    |
| 3   | M     | 4013 | PGE  | O2-C3-C4-O3    |
| 4   | B     | 3002 | GOL  | O1-C1-C2-O2    |
| 3   | I     | 4009 | PGE  | C3-C4-O3-C5    |
| 3   | A     | 4001 | PGE  | C3-C4-O3-C5    |
| 3   | C     | 4003 | PGE  | C3-C4-O3-C5    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | D     | 4004 | PGE  | C3-C4-O3-C5     |
| 3   | L     | 4012 | PGE  | O1-C1-C2-O2     |
| 3   | E     | 4005 | PGE  | C1-C2-O2-C3     |
| 2   | J     | 510  | CMQ  | C12-C11-C9-C10  |
| 3   | I     | 4009 | PGE  | C1-C2-O2-C3     |
| 3   | H     | 4008 | PGE  | C6-C5-O3-C4     |
| 3   | L     | 4012 | PGE  | O2-C3-C4-O3     |
| 3   | F     | 4006 | PGE  | C1-C2-O2-C3     |
| 4   | A     | 3001 | GOL  | O2-C2-C3-O3     |
| 2   | E     | 505  | CMQ  | C9-C11-C12-C14  |
| 3   | G     | 4007 | PGE  | C4-C3-O2-C2     |
| 3   | F     | 4006 | PGE  | C3-C4-O3-C5     |
| 2   | E     | 505  | CMQ  | C12-C11-C9-N1   |
| 3   | C     | 4003 | PGE  | C4-C3-O2-C2     |
| 3   | B     | 4002 | PGE  | O3-C5-C6-O4     |
| 3   | K     | 4015 | PGE  | C1-C2-O2-C3     |
| 2   | H     | 508  | CMQ  | N2-C15-C16-O4   |
| 2   | M     | 513  | CMQ  | C15-C17-C18-C20 |
| 3   | L     | 4012 | PGE  | C4-C3-O2-C2     |
| 3   | N     | 4014 | PGE  | C3-C4-O3-C5     |
| 3   | M     | 4013 | PGE  | C3-C4-O3-C5     |
| 2   | M     | 513  | CMQ  | C15-C17-C18-C19 |
| 3   | K     | 4011 | PGE  | C6-C5-O3-C4     |
| 3   | A     | 4001 | PGE  | O2-C3-C4-O3     |
| 2   | E     | 505  | CMQ  | C15-C17-C18-C19 |
| 2   | D     | 504  | CMQ  | C12-C11-C9-C10  |
| 2   | E     | 505  | CMQ  | C15-C17-C18-C20 |
| 2   | K     | 511  | CMQ  | C15-C17-C18-C19 |
| 3   | N     | 4014 | PGE  | C1-C2-O2-C3     |
| 2   | L     | 512  | CMQ  | C15-C17-C18-C19 |
| 3   | K     | 4015 | PGE  | C3-C4-O3-C5     |
| 2   | N     | 514  | CMQ  | C15-C17-C18-C19 |
| 2   | J     | 510  | CMQ  | C3-C2-O1-C1     |
| 2   | C     | 503  | CMQ  | C15-C17-C18-C20 |
| 2   | L     | 512  | CMQ  | C15-C17-C18-C20 |
| 2   | N     | 514  | CMQ  | C15-C17-C18-C20 |
| 2   | K     | 511  | CMQ  | C15-C17-C18-C20 |
| 2   | C     | 503  | CMQ  | C15-C17-C18-C19 |
| 4   | K     | 3010 | GOL  | O2-C2-C3-O3     |
| 3   | D     | 4004 | PGE  | C1-C2-O2-C3     |
| 2   | B     | 502  | CMQ  | C15-C17-C18-C20 |
| 2   | B     | 502  | CMQ  | C15-C17-C18-C19 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | K     | 4015 | PGE  | C4-C3-O2-C2     |
| 2   | H     | 508  | CMQ  | C15-C17-C18-C20 |
| 3   | K     | 4011 | PGE  | C1-C2-O2-C3     |
| 3   | F     | 4006 | PGE  | O2-C3-C4-O3     |
| 2   | F     | 506  | CMQ  | O2-C1-O1-C2     |
| 3   | D     | 4004 | PGE  | C4-C3-O2-C2     |
| 2   | G     | 507  | CMQ  | C15-C17-C18-C20 |
| 2   | F     | 506  | CMQ  | C15-C17-C18-C20 |
| 2   | H     | 508  | CMQ  | C15-C17-C18-C19 |
| 3   | F     | 4006 | PGE  | C6-C5-O3-C4     |
| 3   | C     | 4003 | PGE  | O1-C1-C2-O2     |
| 2   | N     | 514  | CMQ  | C17-C15-C16-O4  |
| 2   | I     | 509  | CMQ  | C15-C17-C18-C19 |
| 2   | G     | 507  | CMQ  | C15-C17-C18-C19 |
| 2   | G     | 507  | CMQ  | N1-C1-O1-C2     |
| 3   | H     | 4008 | PGE  | O2-C3-C4-O3     |
| 2   | E     | 505  | CMQ  | N2-C15-C16-O4   |
| 2   | J     | 510  | CMQ  | N2-C15-C16-O4   |
| 2   | K     | 511  | CMQ  | N2-C15-C16-O4   |
| 2   | L     | 512  | CMQ  | N2-C15-C16-O4   |
| 2   | L     | 512  | CMQ  | N2-C15-C16-C24  |
| 2   | M     | 513  | CMQ  | N2-C15-C16-O4   |

There are no ring outliers.

28 monomers are involved in 107 short contacts:

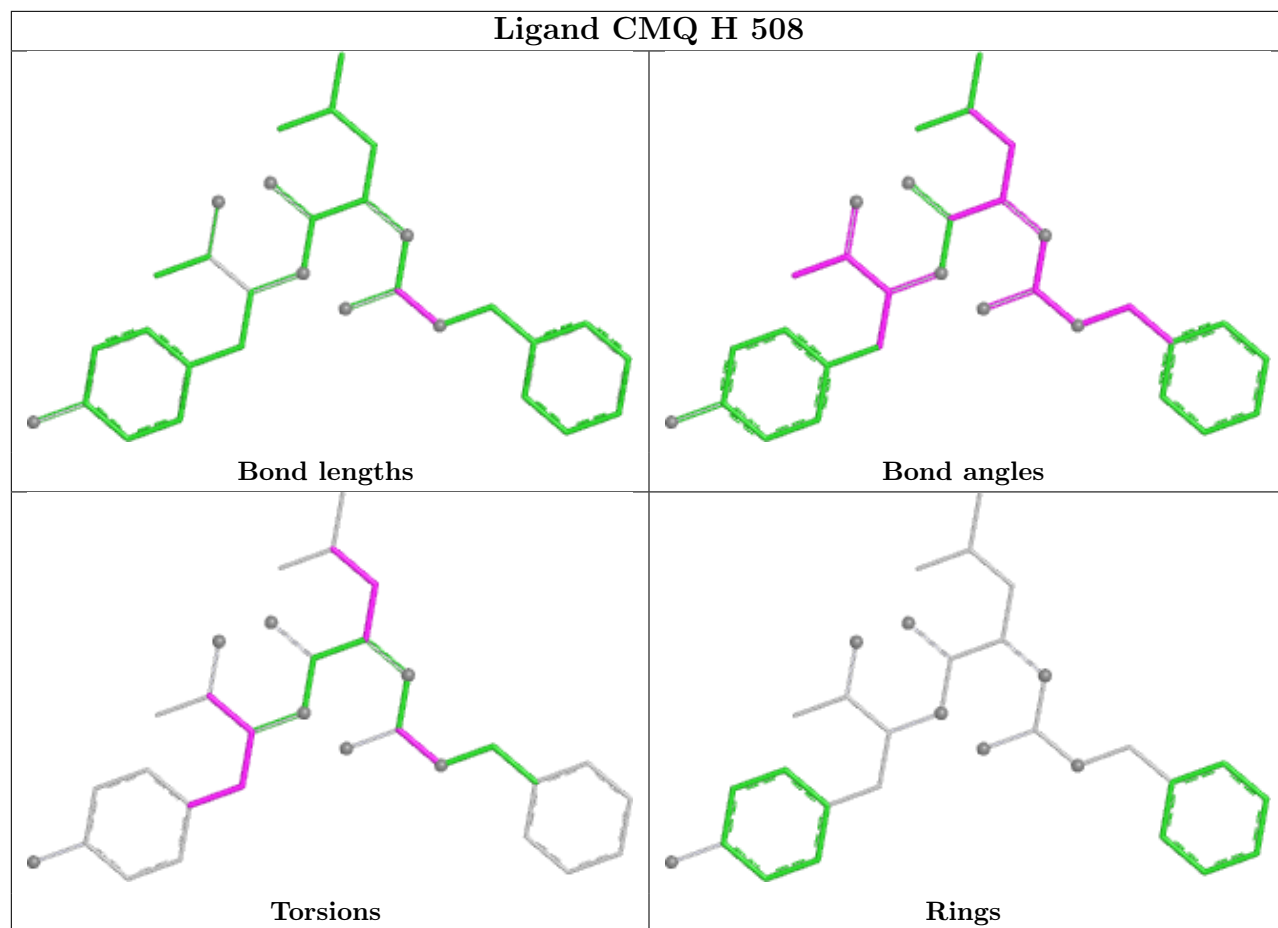
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | H     | 508  | CMQ  | 6       | 0            |
| 3   | B     | 4002 | PGE  | 2       | 0            |
| 3   | A     | 4001 | PGE  | 1       | 0            |
| 4   | G     | 3009 | GOL  | 1       | 0            |
| 2   | G     | 507  | CMQ  | 1       | 0            |
| 4   | N     | 3007 | GOL  | 3       | 0            |
| 4   | A     | 3001 | GOL  | 2       | 0            |
| 4   | H     | 3008 | GOL  | 2       | 0            |
| 3   | F     | 4006 | PGE  | 1       | 0            |
| 2   | J     | 510  | CMQ  | 8       | 0            |
| 2   | B     | 502  | CMQ  | 7       | 0            |
| 2   | C     | 503  | CMQ  | 6       | 0            |
| 2   | A     | 501  | CMQ  | 9       | 0            |
| 2   | E     | 505  | CMQ  | 8       | 0            |
| 2   | N     | 514  | CMQ  | 2       | 0            |

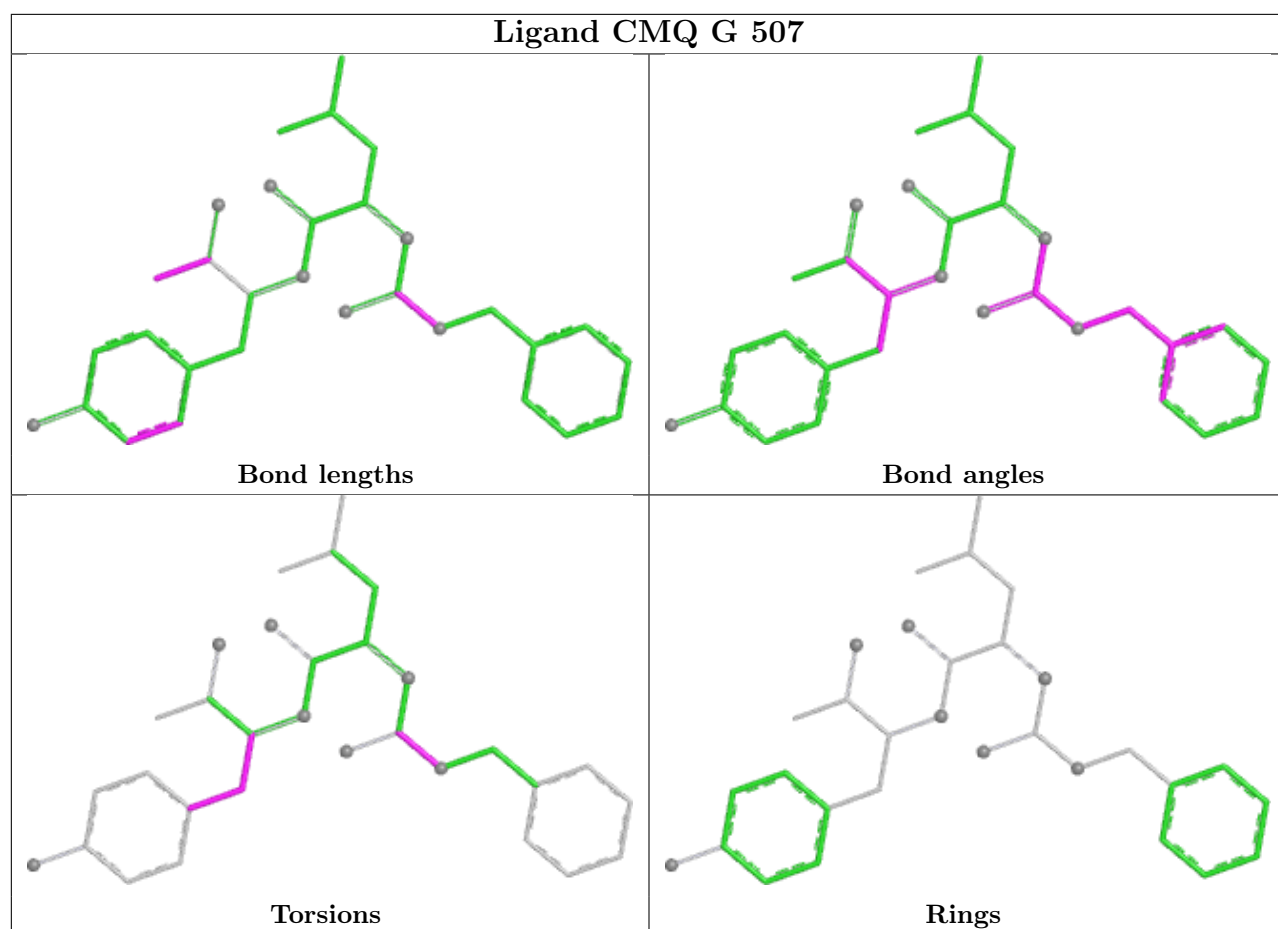
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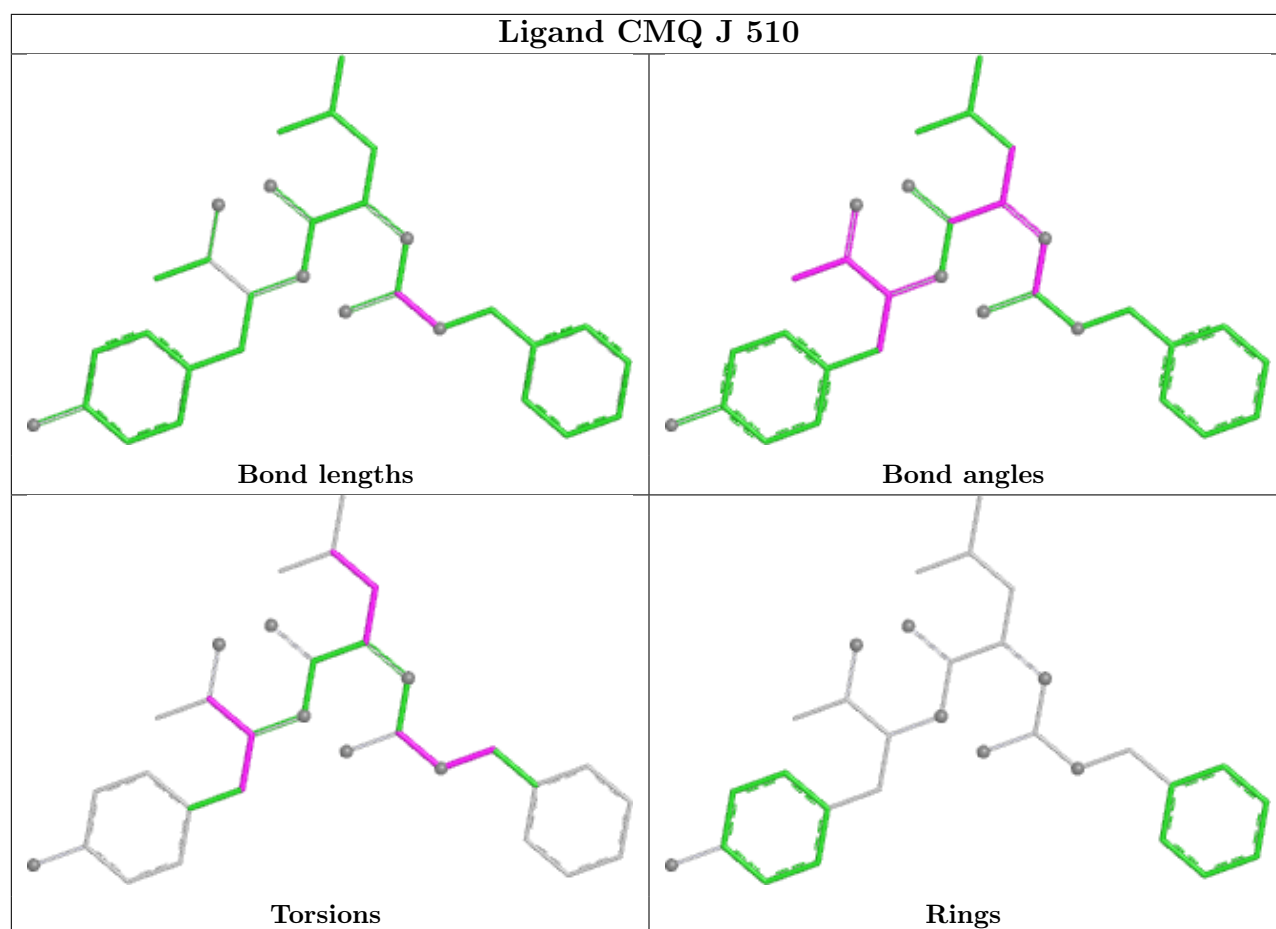
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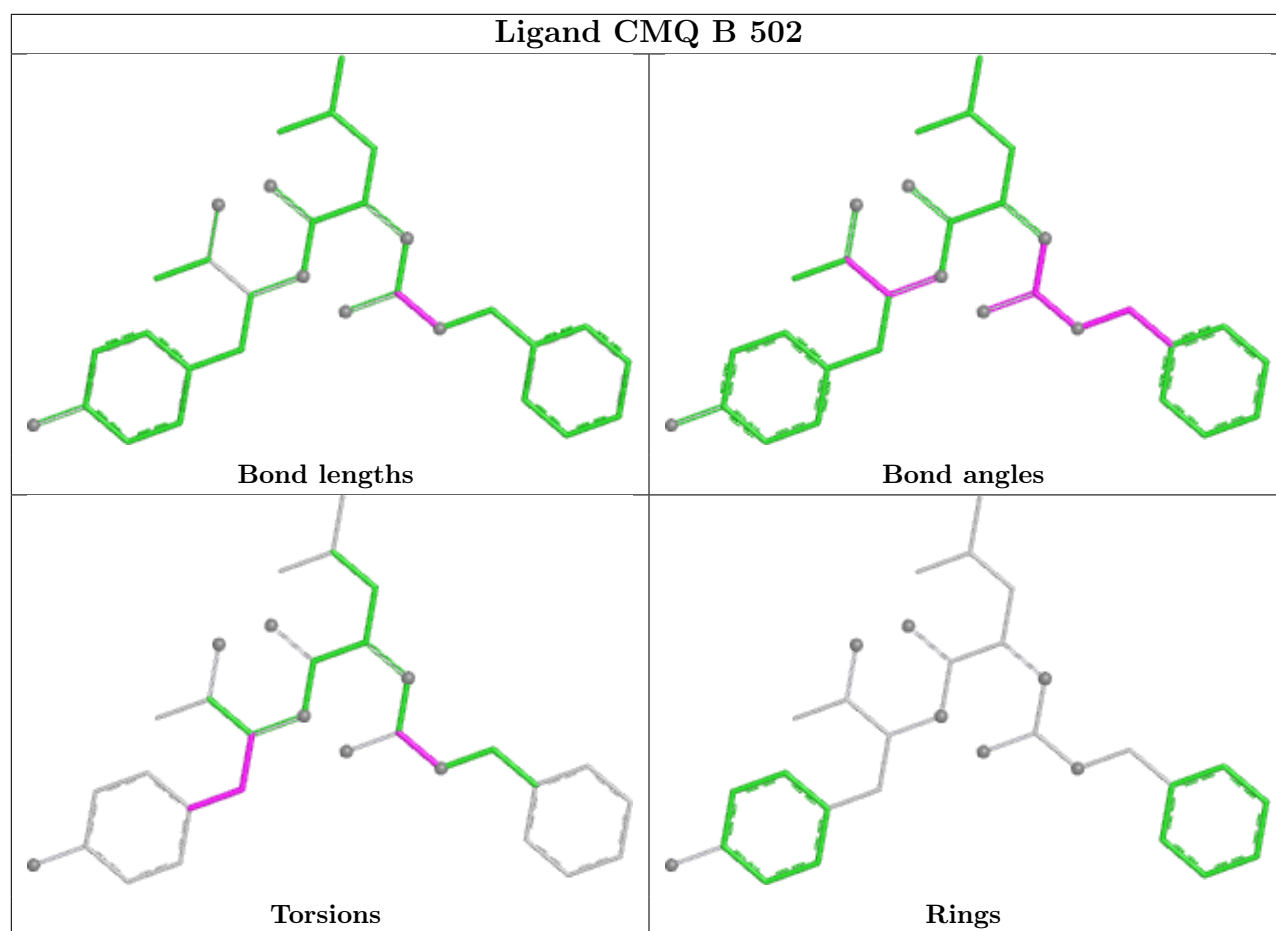
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | M     | 513  | CMQ  | 1       | 0            |
| 2   | D     | 504  | CMQ  | 8       | 0            |
| 2   | L     | 512  | CMQ  | 7       | 0            |
| 4   | K     | 3010 | GOL  | 1       | 0            |
| 4   | C     | 3006 | GOL  | 6       | 0            |
| 3   | J     | 4010 | PGE  | 1       | 0            |
| 4   | F     | 3004 | GOL  | 2       | 0            |
| 2   | F     | 506  | CMQ  | 1       | 0            |
| 3   | N     | 4014 | PGE  | 2       | 0            |
| 2   | K     | 511  | CMQ  | 9       | 0            |
| 3   | K     | 4015 | PGE  | 2       | 0            |
| 3   | M     | 4013 | PGE  | 1       | 0            |
| 2   | I     | 509  | CMQ  | 7       | 0            |

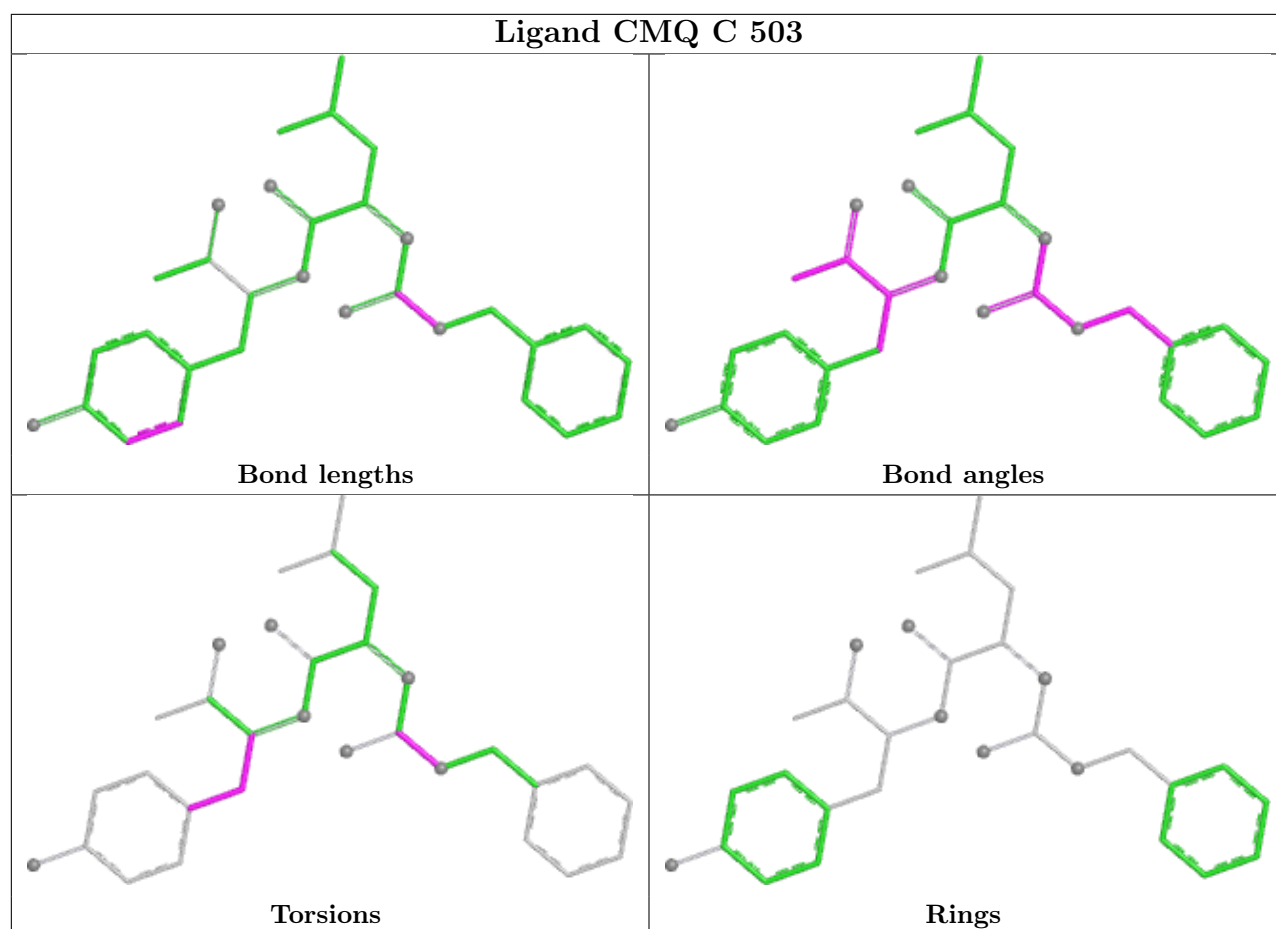
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

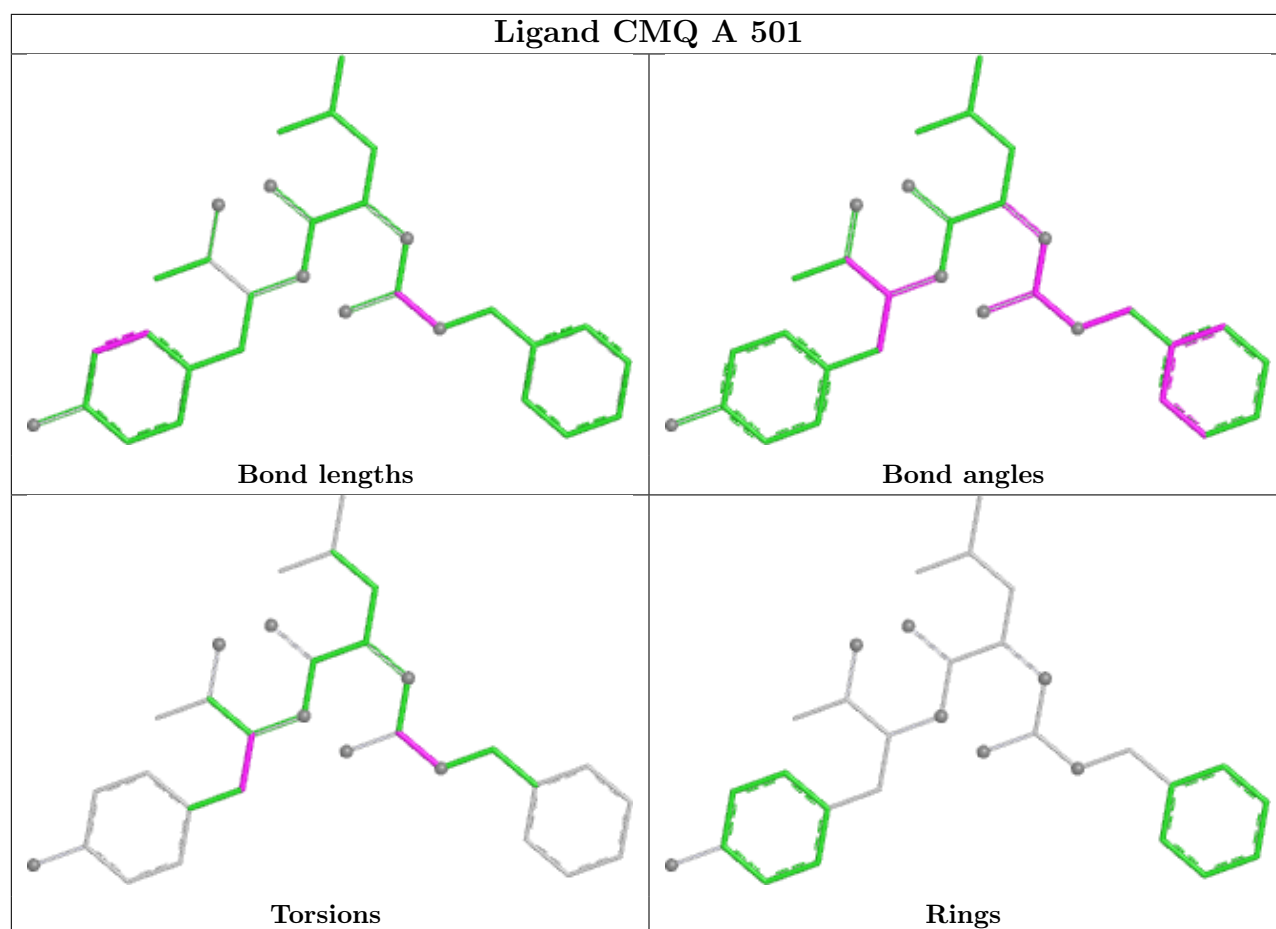


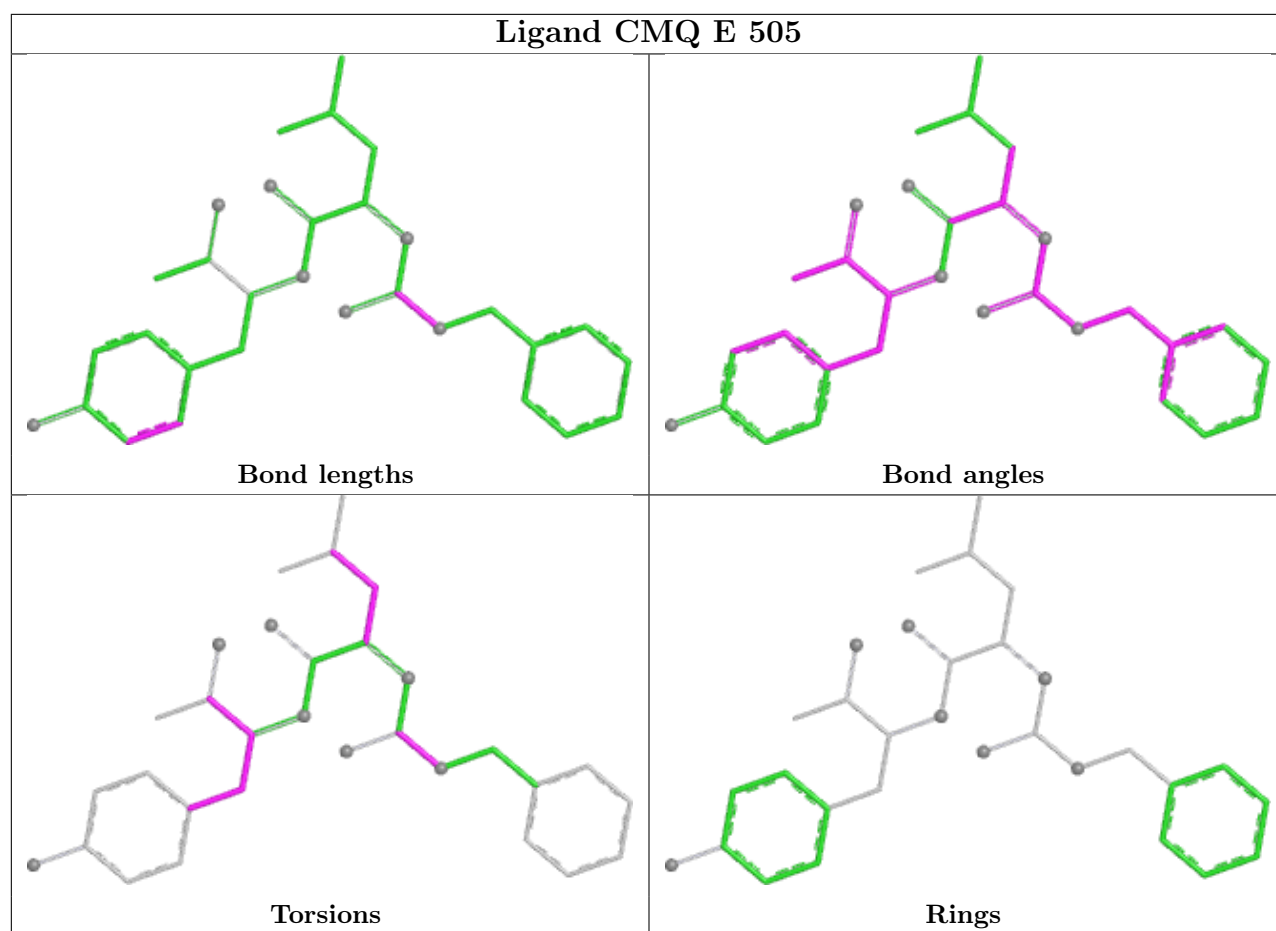


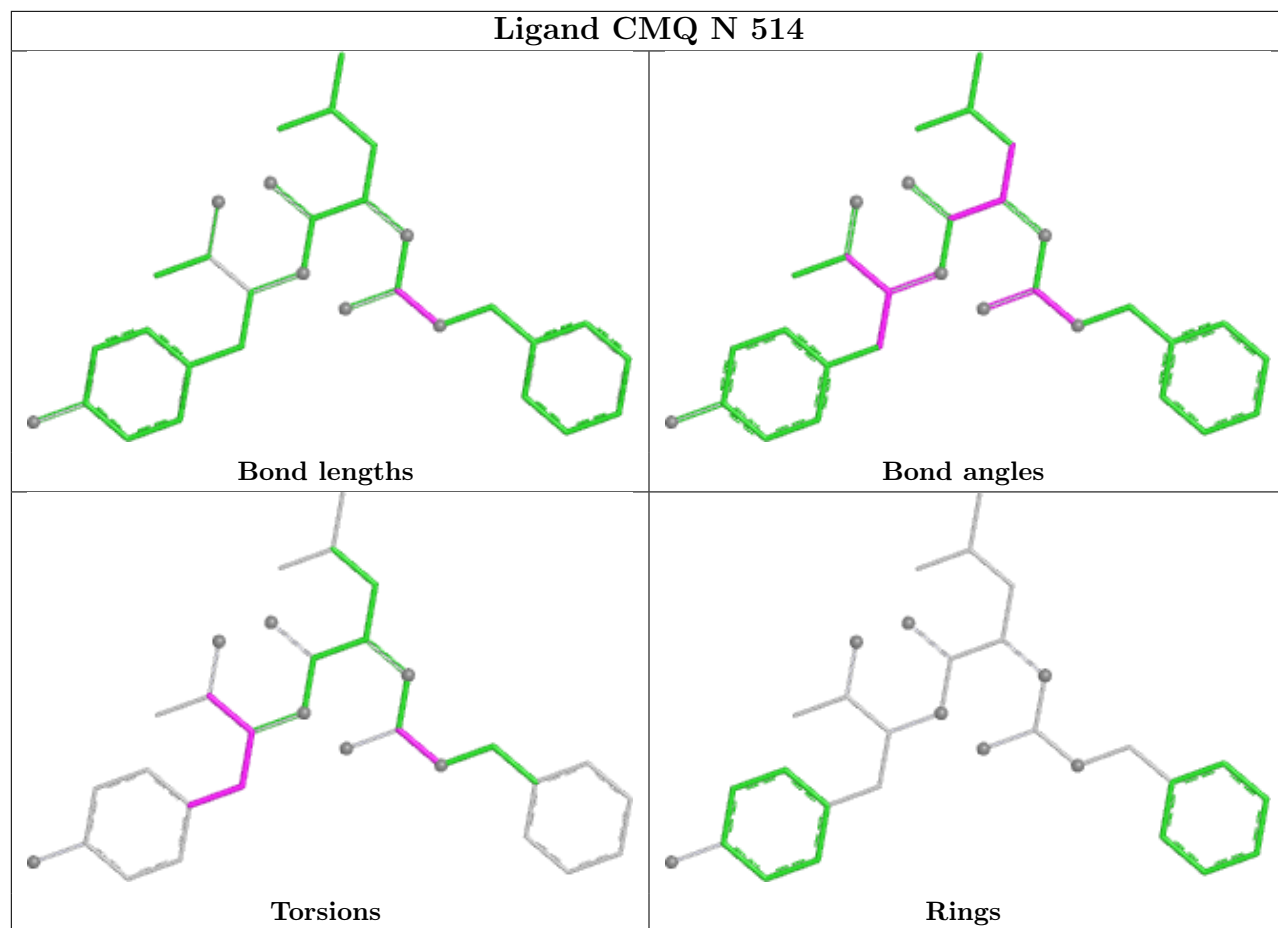




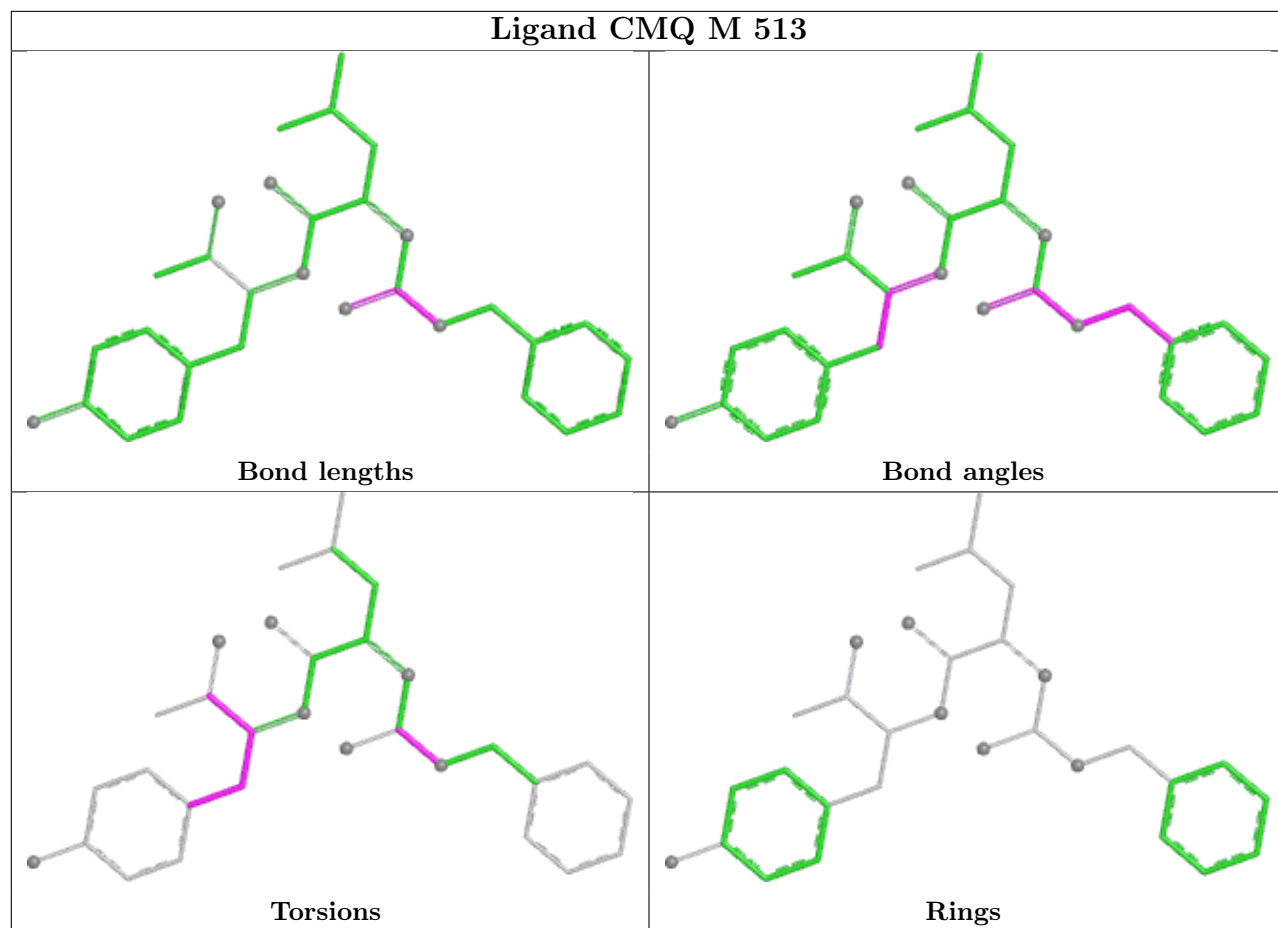


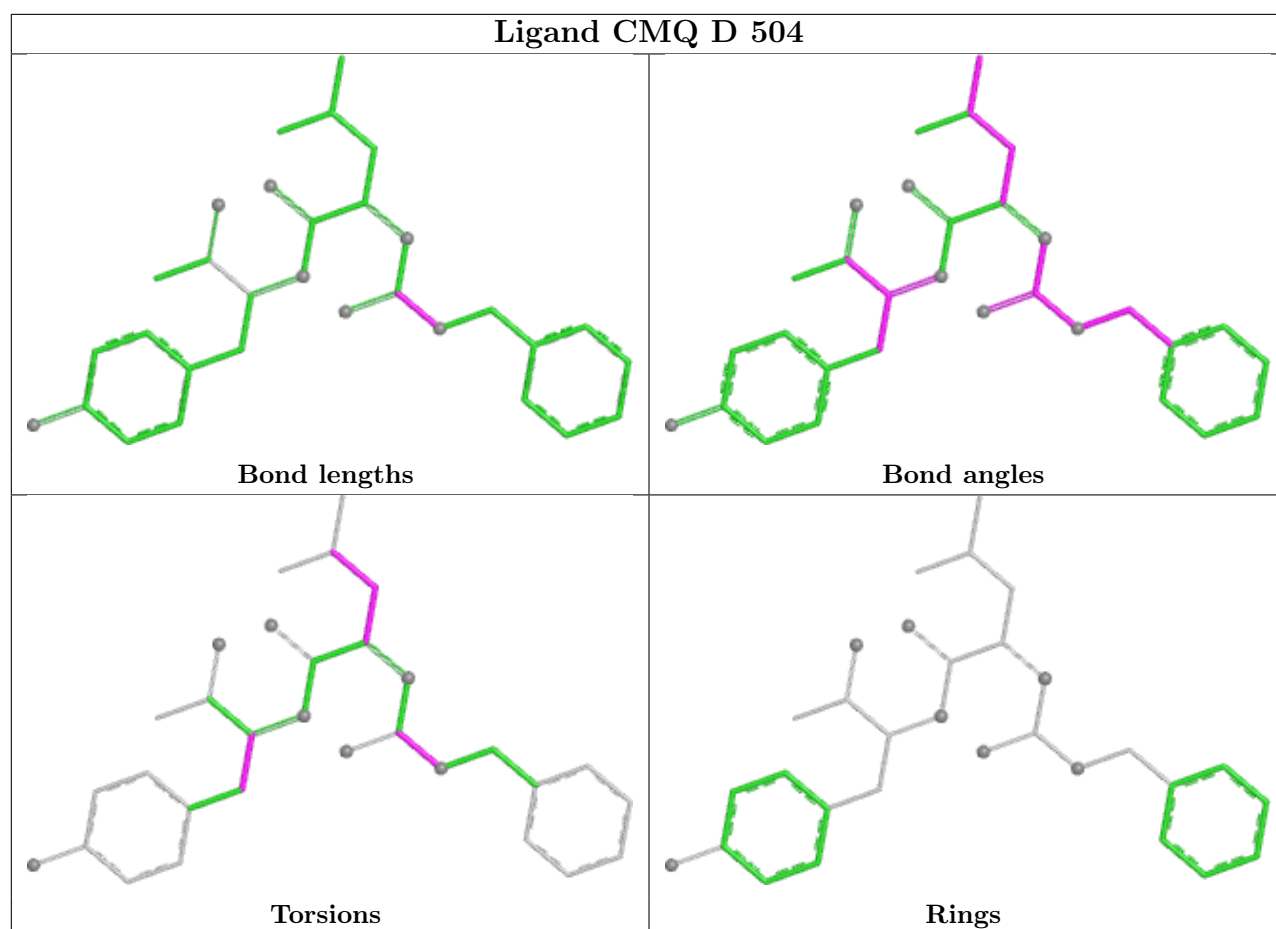


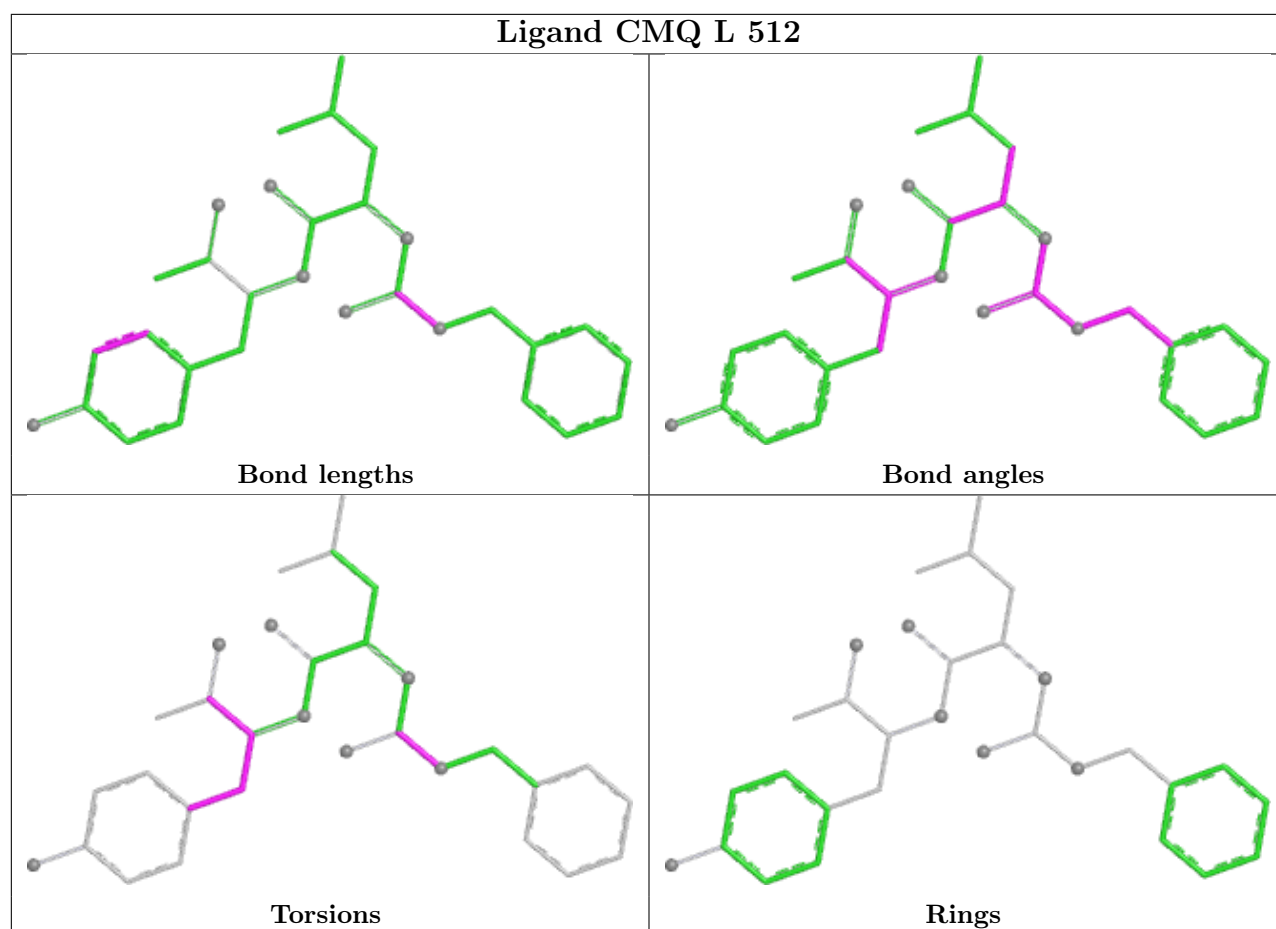


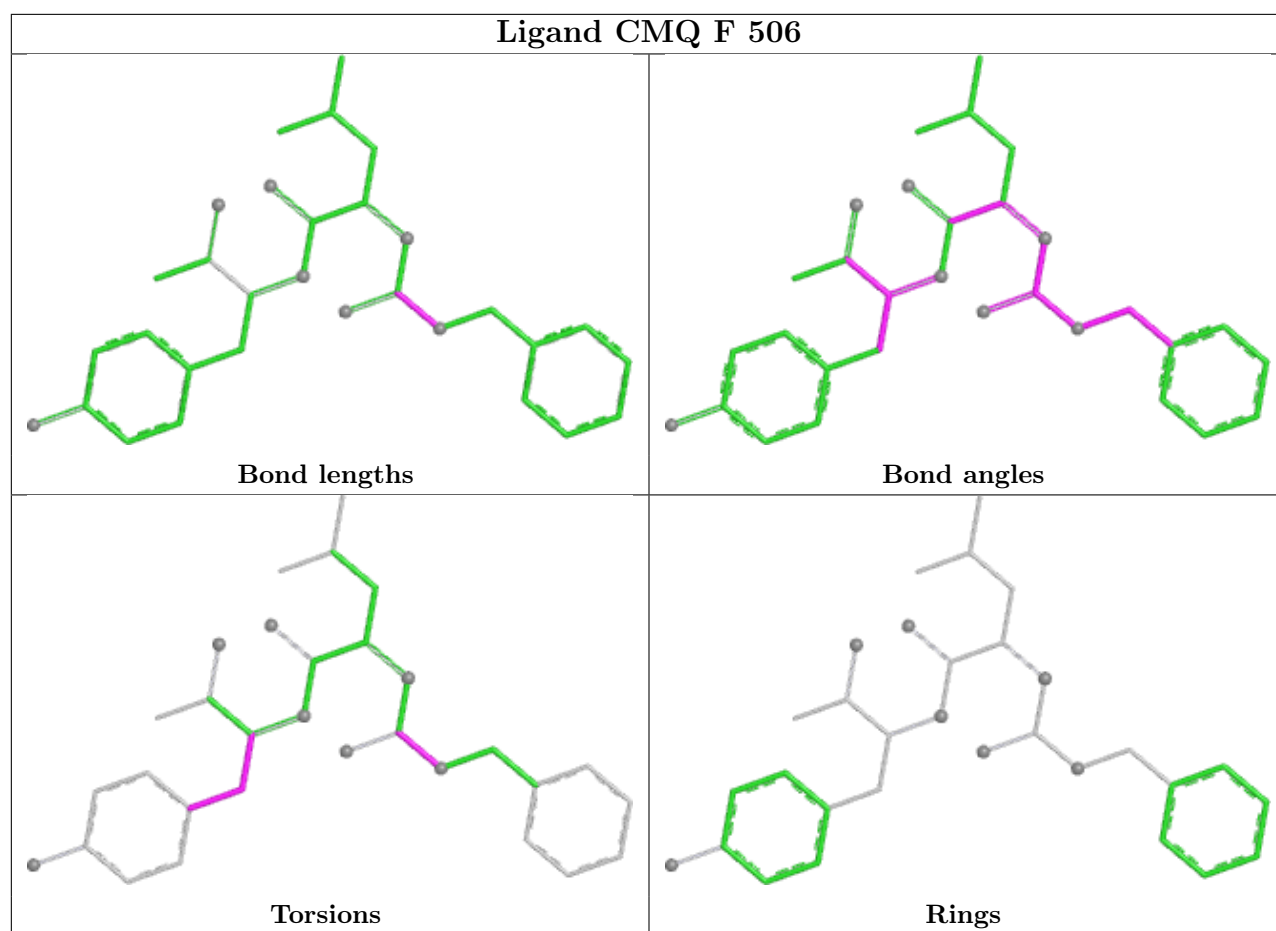


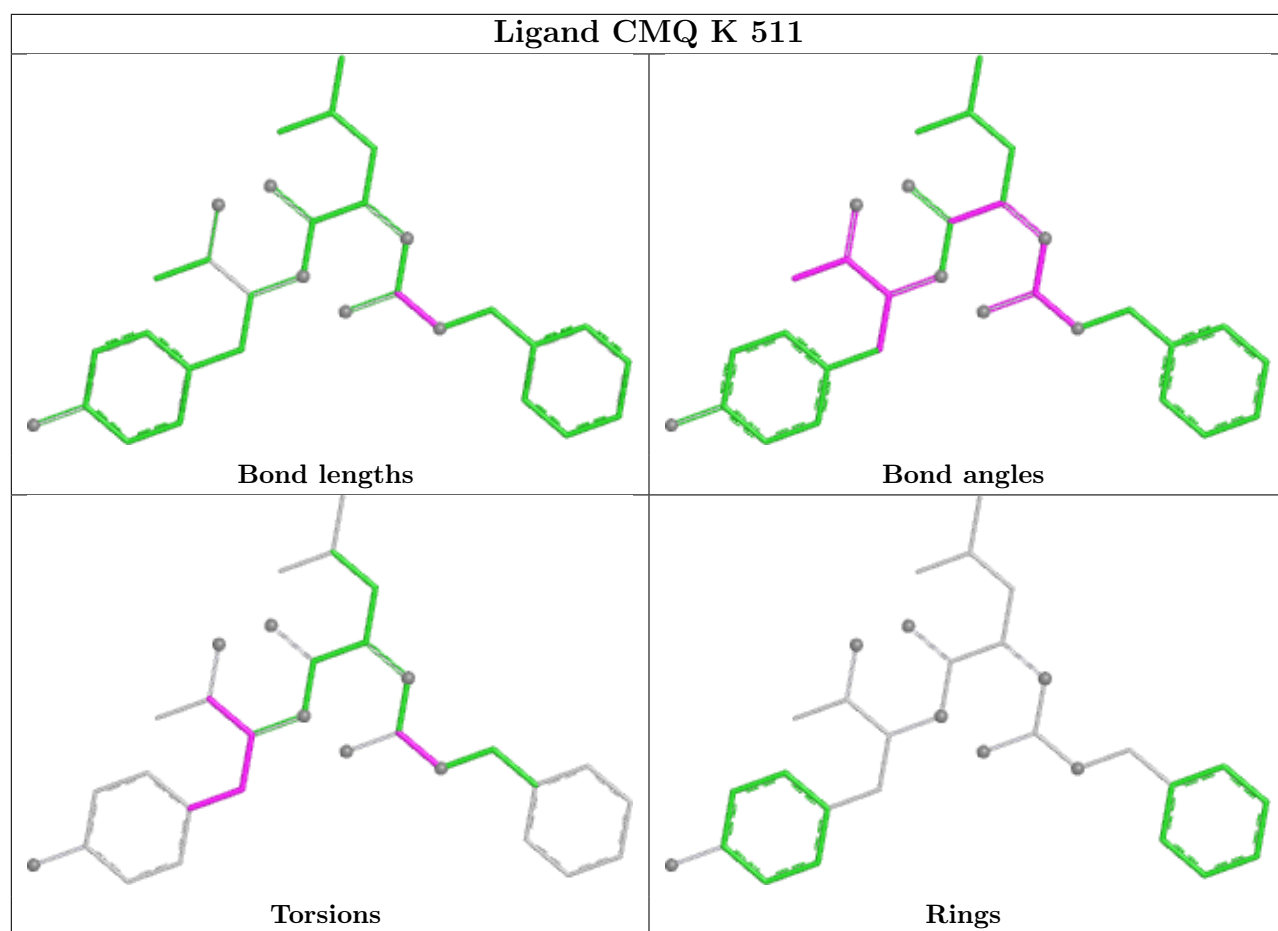
## Ligand CMQ M 513

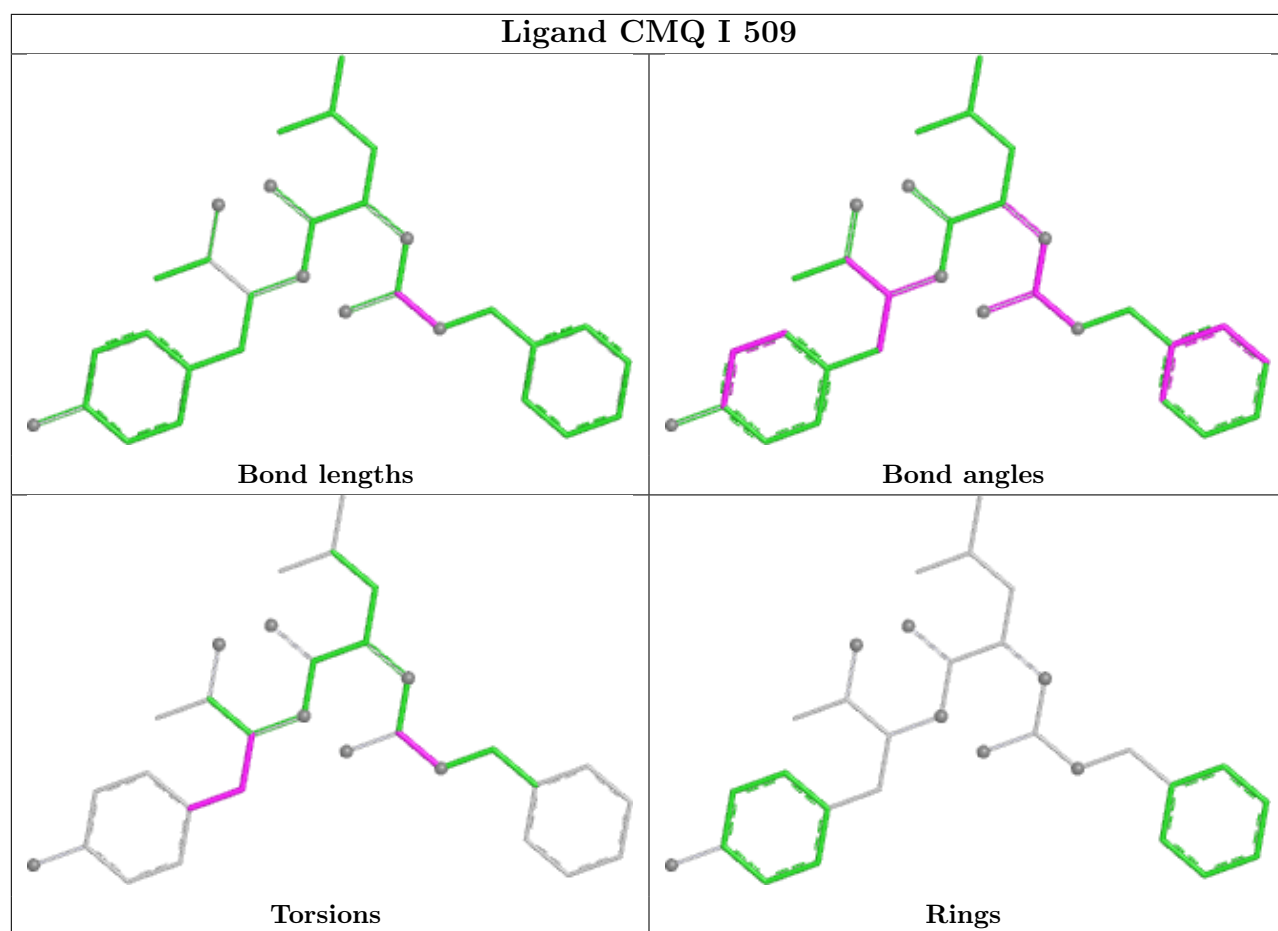












## 5.7 Other polymers [i](#)

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     | 186/193 (96%)   | 0.55   | 9 (4%) 35 38   | 20, 32, 50, 69        | 7 (3%)  |
| 1   | B     | 192/193 (99%)   | 0.89   | 27 (14%) 6 6   | 21, 33, 53, 69        | 10 (5%) |
| 1   | C     | 183/193 (94%)   | 0.76   | 14 (7%) 19 21  | 20, 33, 43, 66        | 7 (3%)  |
| 1   | D     | 185/193 (95%)   | 0.72   | 16 (8%) 16 17  | 20, 33, 52, 72        | 3 (1%)  |
| 1   | E     | 188/193 (97%)   | 0.98   | 24 (12%) 7 8   | 22, 32, 50, 66        | 2 (1%)  |
| 1   | F     | 185/193 (95%)   | 0.51   | 10 (5%) 31 33  | 21, 32, 46, 59        | 2 (1%)  |
| 1   | G     | 183/193 (94%)   | 0.53   | 8 (4%) 39 41   | 20, 32, 46, 68        | 4 (2%)  |
| 1   | H     | 183/193 (94%)   | 0.49   | 9 (4%) 35 37   | 21, 32, 46, 78        | 2 (1%)  |
| 1   | I     | 183/193 (94%)   | 0.54   | 7 (3%) 44 47   | 17, 32, 43, 64        | 7 (3%)  |
| 1   | J     | 185/193 (95%)   | 0.56   | 10 (5%) 31 33  | 21, 32, 48, 79        | 2 (1%)  |
| 1   | K     | 186/193 (96%)   | 0.55   | 11 (5%) 28 30  | 20, 33, 53, 70        | 1 (0%)  |
| 1   | L     | 183/193 (94%)   | 0.55   | 8 (4%) 39 41   | 20, 32, 45, 68        | 11 (6%) |
| 1   | M     | 186/193 (96%)   | 0.62   | 12 (6%) 25 26  | 20, 32, 52, 70        | 11 (5%) |
| 1   | N     | 183/193 (94%)   | 0.50   | 10 (5%) 30 32  | 20, 32, 44, 73        | 10 (5%) |
| All | All   | 2591/2702 (95%) | 0.63   | 175 (6%) 23 24 | 17, 33, 51, 79        | 79 (3%) |

All (175) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | M     | 1   | ALA  | 7.7  |
| 1   | G     | 16  | SER  | 7.2  |
| 1   | G     | 5   | MET  | 7.1  |
| 1   | F     | 16  | SER  | 6.7  |
| 1   | G     | 6   | VAL  | 6.5  |
| 1   | G     | 17  | PHE  | 6.5  |
| 1   | C     | 6   | VAL  | 6.4  |
| 1   | L     | 17  | PHE  | 6.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 17  | PHE  | 6.3  |
| 1   | A     | 193 | ASN  | 6.1  |
| 1   | N     | 17  | PHE  | 6.0  |
| 1   | C     | 5   | MET  | 5.5  |
| 1   | F     | 7   | ILE  | 5.4  |
| 1   | I     | 16  | SER  | 5.3  |
| 1   | G     | 2   | LEU  | 5.3  |
| 1   | A     | 7   | ILE  | 5.3  |
| 1   | C     | 193 | ASN  | 5.2  |
| 1   | E     | 193 | ASN  | 5.2  |
| 1   | D     | 2   | LEU  | 5.2  |
| 1   | L     | 5   | MET  | 5.2  |
| 1   | J     | 193 | ASN  | 5.1  |
| 1   | H     | 17  | PHE  | 5.1  |
| 1   | I     | 17  | PHE  | 5.1  |
| 1   | L     | 2   | LEU  | 4.9  |
| 1   | M     | 7   | ILE  | 4.8  |
| 1   | B     | 16  | SER  | 4.7  |
| 1   | F     | 2   | LEU  | 4.7  |
| 1   | M     | 17  | PHE  | 4.7  |
| 1   | M     | 193 | ASN  | 4.6  |
| 1   | D     | 17  | PHE  | 4.6  |
| 1   | H     | 2   | LEU  | 4.6  |
| 1   | I     | 2   | LEU  | 4.6  |
| 1   | B     | 193 | ASN  | 4.6  |
| 1   | F     | 17  | PHE  | 4.5  |
| 1   | A     | 17  | PHE  | 4.5  |
| 1   | K     | 17  | PHE  | 4.4  |
| 1   | L     | 3   | VAL  | 4.3  |
| 1   | G     | 3   | VAL  | 4.3  |
| 1   | F     | 193 | ASN  | 4.3  |
| 1   | E     | 6   | VAL  | 4.2  |
| 1   | E     | 15  | ARG  | 4.2  |
| 1   | J     | 7   | ILE  | 4.2  |
| 1   | D     | 193 | ASN  | 4.2  |
| 1   | K     | 16  | SER  | 4.1  |
| 1   | I     | 193 | ASN  | 4.1  |
| 1   | D     | 6   | VAL  | 4.0  |
| 1   | L     | 16  | SER  | 4.0  |
| 1   | E     | 133 | THR  | 4.0  |
| 1   | J     | 2   | LEU  | 4.0  |
| 1   | B     | 17  | PHE  | 4.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 16  | SER  | 4.0  |
| 1   | N     | 2   | LEU  | 4.0  |
| 1   | N     | 6   | VAL  | 4.0  |
| 1   | D     | 5   | MET  | 3.9  |
| 1   | E     | 7   | ILE  | 3.9  |
| 1   | C     | 17  | PHE  | 3.9  |
| 1   | M     | 2   | LEU  | 3.9  |
| 1   | B     | 2   | LEU  | 3.8  |
| 1   | M     | 15  | ARG  | 3.8  |
| 1   | K     | 193 | ASN  | 3.8  |
| 1   | B     | 135 | ILE  | 3.8  |
| 1   | E     | 17  | PHE  | 3.8  |
| 1   | C     | 15  | ARG  | 3.7  |
| 1   | G     | 193 | ASN  | 3.7  |
| 1   | E     | 5   | MET  | 3.6  |
| 1   | J     | 16  | SER  | 3.6  |
| 1   | K     | 2   | LEU  | 3.6  |
| 1   | A     | 2   | LEU  | 3.6  |
| 1   | F     | 3   | VAL  | 3.5  |
| 1   | F     | 6   | VAL  | 3.5  |
| 1   | H     | 193 | ASN  | 3.5  |
| 1   | H     | 3   | VAL  | 3.4  |
| 1   | L     | 6   | VAL  | 3.3  |
| 1   | D     | 16  | SER  | 3.3  |
| 1   | D     | 185 | VAL  | 3.2  |
| 1   | M     | 6   | VAL  | 3.2  |
| 1   | B     | 137 | ILE  | 3.2  |
| 1   | E     | 2   | LEU  | 3.2  |
| 1   | K     | 15  | ARG  | 3.2  |
| 1   | B     | 10  | THR  | 3.1  |
| 1   | B     | 11  | SER  | 3.1  |
| 1   | C     | 3   | VAL  | 3.1  |
| 1   | E     | 9   | GLN  | 3.1  |
| 1   | D     | 133 | THR  | 3.1  |
| 1   | N     | 16  | SER  | 3.1  |
| 1   | D     | 137 | ILE  | 3.1  |
| 1   | E     | 3   | VAL  | 3.1  |
| 1   | F     | 5   | MET  | 3.1  |
| 1   | N     | 193 | ASN  | 3.1  |
| 1   | B     | 132 | ALA  | 3.1  |
| 1   | F     | 15  | ARG  | 3.0  |
| 1   | A     | 128 | TYR  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 15  | ARG  | 3.0  |
| 1   | B     | 7   | ILE  | 3.0  |
| 1   | D     | 135 | ILE  | 3.0  |
| 1   | C     | 135 | ILE  | 2.9  |
| 1   | B     | 14  | GLU  | 2.9  |
| 1   | B     | 6   | VAL  | 2.9  |
| 1   | C     | 129 | GLN  | 2.9  |
| 1   | M     | 5   | MET  | 2.9  |
| 1   | K     | 6   | VAL  | 2.8  |
| 1   | K     | 3   | VAL  | 2.8  |
| 1   | N     | 3   | VAL  | 2.8  |
| 1   | K     | 7   | ILE  | 2.8  |
| 1   | J     | 5   | MET  | 2.8  |
| 1   | A     | 16  | SER  | 2.8  |
| 1   | E     | 16  | SER  | 2.8  |
| 1   | B     | 9   | GLN  | 2.8  |
| 1   | C     | 4   | PRO  | 2.8  |
| 1   | D     | 132 | ALA  | 2.7  |
| 1   | M     | 16  | SER  | 2.7  |
| 1   | E     | 14  | GLU  | 2.7  |
| 1   | E     | 25  | LYS  | 2.7  |
| 1   | A     | 191 | HIS  | 2.7  |
| 1   | D     | 7   | ILE  | 2.7  |
| 1   | C     | 126 | GLY  | 2.7  |
| 1   | N     | 5   | MET  | 2.7  |
| 1   | B     | 13  | GLY  | 2.6  |
| 1   | B     | 133 | THR  | 2.6  |
| 1   | J     | 8   | GLU  | 2.6  |
| 1   | L     | 193 | ASN  | 2.6  |
| 1   | J     | 3   | VAL  | 2.6  |
| 1   | A     | 15  | ARG  | 2.6  |
| 1   | B     | 129 | GLN  | 2.6  |
| 1   | J     | 6   | VAL  | 2.6  |
| 1   | N     | 56  | GLU  | 2.5  |
| 1   | I     | 6   | VAL  | 2.5  |
| 1   | C     | 137 | ILE  | 2.5  |
| 1   | E     | 137 | ILE  | 2.5  |
| 1   | E     | 132 | ALA  | 2.5  |
| 1   | I     | 132 | ALA  | 2.5  |
| 1   | H     | 6   | VAL  | 2.5  |
| 1   | N     | 129 | GLN  | 2.4  |
| 1   | H     | 16  | SER  | 2.4  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | B     | 5      | MET  | 2.4  |
| 1   | K     | 8      | GLU  | 2.4  |
| 1   | B     | 32     | THR  | 2.4  |
| 1   | E     | 135    | ILE  | 2.4  |
| 1   | C     | 132    | ALA  | 2.4  |
| 1   | E     | 130    | GLY  | 2.4  |
| 1   | B     | 125    | LEU  | 2.3  |
| 1   | D     | 129[A] | GLN  | 2.3  |
| 1   | I     | 5      | MET  | 2.3  |
| 1   | E     | 145    | VAL  | 2.3  |
| 1   | E     | 142    | ILE  | 2.3  |
| 1   | K     | 5      | MET  | 2.3  |
| 1   | B     | 69     | VAL  | 2.3  |
| 1   | M     | 133    | THR  | 2.3  |
| 1   | H     | 4      | PRO  | 2.2  |
| 1   | E     | 129    | GLN  | 2.2  |
| 1   | E     | 190    | THR  | 2.2  |
| 1   | B     | 143    | LEU  | 2.2  |
| 1   | M     | 128    | TYR  | 2.2  |
| 1   | J     | 84     | LYS  | 2.2  |
| 1   | M     | 3      | VAL  | 2.2  |
| 1   | E     | 143    | LEU  | 2.2  |
| 1   | D     | 139    | ALA  | 2.2  |
| 1   | F     | 166    | ARG  | 2.2  |
| 1   | A     | 8      | GLU  | 2.1  |
| 1   | B     | 131    | GLN  | 2.1  |
| 1   | B     | 130    | GLY  | 2.1  |
| 1   | D     | 166    | ARG  | 2.1  |
| 1   | N     | 4      | PRO  | 2.1  |
| 1   | D     | 8      | GLU  | 2.1  |
| 1   | E     | 56     | GLU  | 2.1  |
| 1   | H     | 128    | TYR  | 2.1  |
| 1   | B     | 126    | GLY  | 2.1  |
| 1   | G     | 166    | ARG  | 2.1  |
| 1   | H     | 5      | MET  | 2.0  |
| 1   | C     | 139    | ALA  | 2.0  |
| 1   | E     | 139    | ALA  | 2.0  |
| 1   | B     | 8      | GLU  | 2.0  |
| 1   | K     | 19     | ILE  | 2.0  |
| 1   | B     | 128    | TYR  | 2.0  |
| 1   | L     | 128    | TYR  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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.

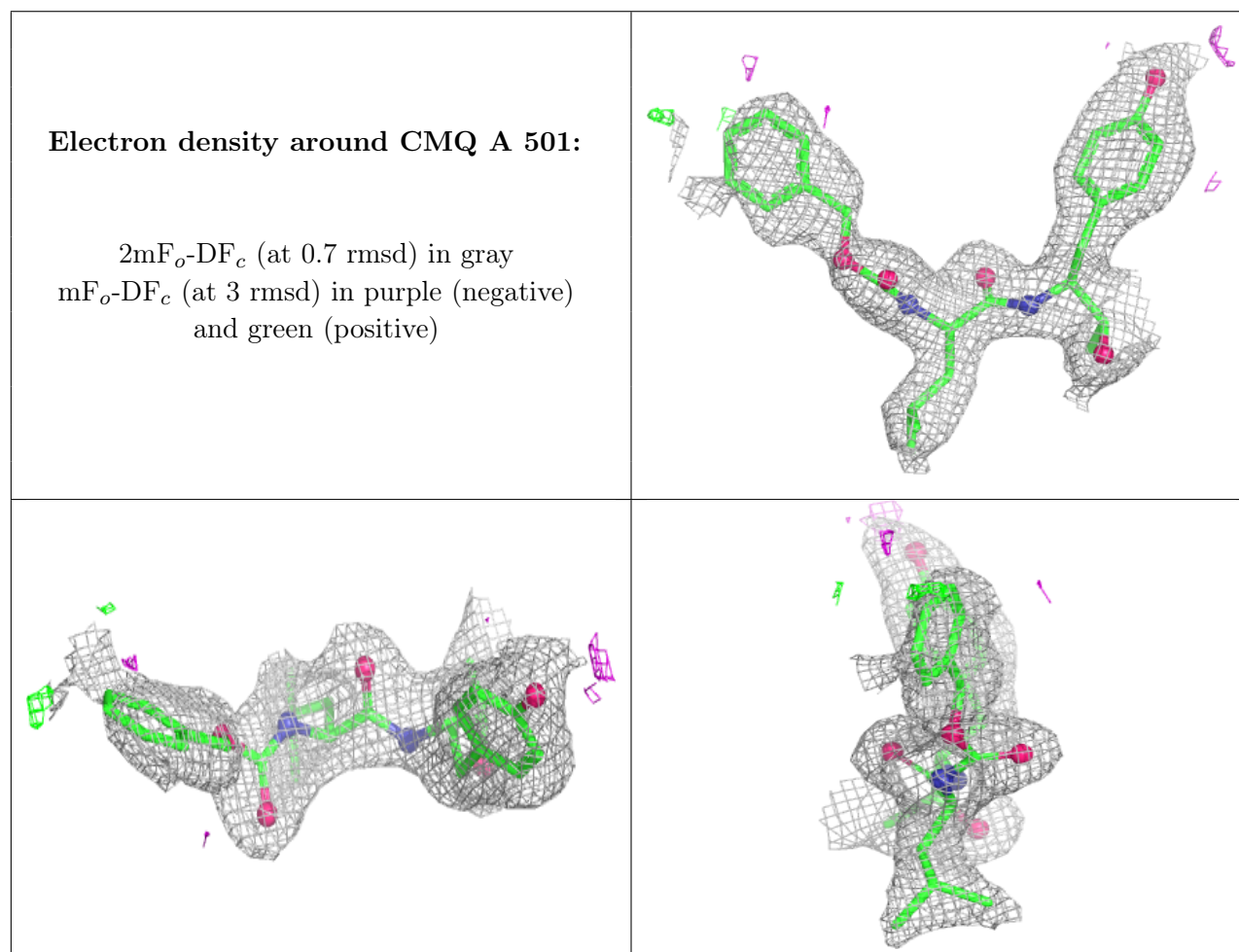
| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | PGE  | C     | 4003 | 10/10 | 0.70 | 0.12 | 63,64,66,66                 | 0     |
| 3   | PGE  | N     | 4014 | 10/10 | 0.71 | 0.12 | 59,65,69,70                 | 0     |
| 3   | PGE  | B     | 4002 | 10/10 | 0.72 | 0.12 | 61,62,63,64                 | 0     |
| 4   | GOL  | B     | 3002 | 6/6   | 0.72 | 0.12 | 52,54,56,56                 | 0     |
| 3   | PGE  | K     | 4011 | 10/10 | 0.73 | 0.11 | 48,51,57,59                 | 0     |
| 4   | GOL  | H     | 3008 | 6/6   | 0.73 | 0.12 | 53,55,57,58                 | 0     |
| 3   | PGE  | E     | 4005 | 10/10 | 0.75 | 0.11 | 59,60,63,63                 | 0     |
| 3   | PGE  | H     | 4008 | 10/10 | 0.75 | 0.12 | 52,55,58,59                 | 0     |
| 4   | GOL  | C     | 3006 | 6/6   | 0.76 | 0.12 | 60,62,63,64                 | 0     |
| 3   | PGE  | J     | 4010 | 10/10 | 0.76 | 0.12 | 41,46,51,52                 | 0     |
| 4   | GOL  | K     | 3010 | 6/6   | 0.77 | 0.20 | 43,46,46,46                 | 0     |
| 4   | GOL  | C     | 3005 | 6/6   | 0.78 | 0.11 | 53,55,56,56                 | 0     |
| 3   | PGE  | D     | 4004 | 10/10 | 0.79 | 0.10 | 55,57,58,60                 | 0     |
| 3   | PGE  | K     | 4015 | 10/10 | 0.80 | 0.12 | 37,40,42,45                 | 0     |
| 3   | PGE  | A     | 4001 | 10/10 | 0.82 | 0.10 | 43,46,50,50                 | 0     |
| 3   | PGE  | I     | 4009 | 10/10 | 0.84 | 0.10 | 48,52,60,60                 | 0     |
| 4   | GOL  | N     | 3007 | 6/6   | 0.84 | 0.14 | 44,48,50,50                 | 0     |
| 4   | GOL  | F     | 3004 | 6/6   | 0.85 | 0.16 | 30,33,34,40                 | 0     |
| 4   | GOL  | B     | 3003 | 6/6   | 0.85 | 0.10 | 56,58,58,60                 | 0     |
| 3   | PGE  | G     | 4007 | 10/10 | 0.85 | 0.10 | 36,39,44,44                 | 0     |
| 3   | PGE  | L     | 4012 | 10/10 | 0.85 | 0.09 | 45,46,49,50                 | 0     |
| 4   | GOL  | G     | 3009 | 6/6   | 0.86 | 0.15 | 42,46,48,49                 | 0     |
| 3   | PGE  | F     | 4006 | 10/10 | 0.86 | 0.09 | 41,43,49,50                 | 0     |
| 2   | CMQ  | A     | 501  | 31/31 | 0.87 | 0.11 | 36,41,56,58                 | 0     |
| 3   | PGE  | M     | 4013 | 10/10 | 0.87 | 0.09 | 43,45,49,54                 | 0     |
| 2   | CMQ  | I     | 509  | 31/31 | 0.87 | 0.11 | 35,41,55,58                 | 0     |
| 4   | GOL  | L     | 3011 | 6/6   | 0.87 | 0.14 | 30,36,38,42                 | 0     |

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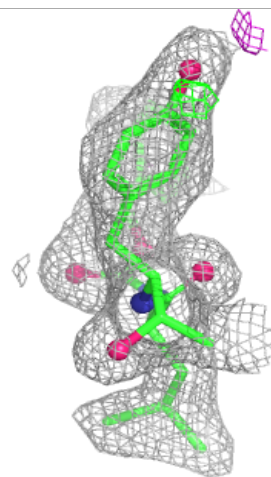
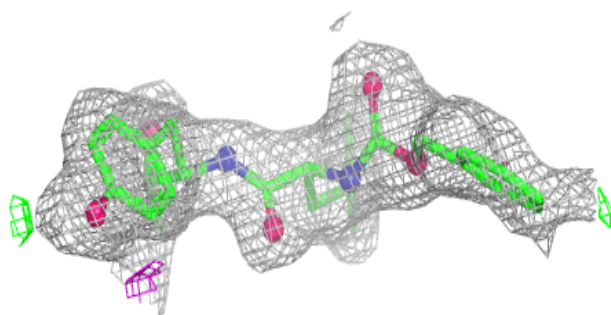
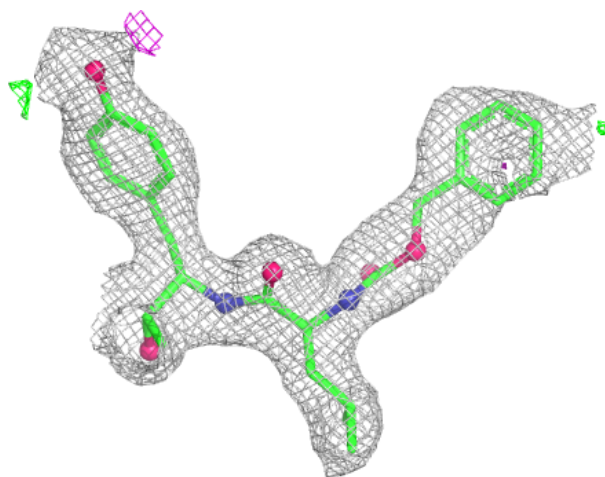
| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2   | CMQ  | K     | 511  | 31/31 | 0.87 | 0.11 | 36,40,56,57                 | 0     |
| 2   | CMQ  | N     | 514  | 31/31 | 0.88 | 0.11 | 34,41,59,60                 | 0     |
| 2   | CMQ  | E     | 505  | 31/31 | 0.88 | 0.12 | 33,39,59,60                 | 0     |
| 2   | CMQ  | H     | 508  | 31/31 | 0.89 | 0.10 | 33,39,62,63                 | 0     |
| 2   | CMQ  | C     | 503  | 31/31 | 0.89 | 0.10 | 34,40,56,58                 | 0     |
| 2   | CMQ  | J     | 510  | 31/31 | 0.89 | 0.09 | 36,41,53,54                 | 0     |
| 2   | CMQ  | B     | 502  | 31/31 | 0.89 | 0.12 | 33,42,58,59                 | 0     |
| 2   | CMQ  | F     | 506  | 31/31 | 0.89 | 0.10 | 34,40,58,59                 | 0     |
| 2   | CMQ  | M     | 513  | 31/31 | 0.90 | 0.10 | 33,39,54,55                 | 0     |
| 2   | CMQ  | D     | 504  | 31/31 | 0.91 | 0.10 | 34,38,55,56                 | 0     |
| 4   | GOL  | A     | 3001 | 6/6   | 0.91 | 0.14 | 32,35,37,42                 | 0     |
| 2   | CMQ  | L     | 512  | 31/31 | 0.91 | 0.12 | 35,40,62,64                 | 0     |
| 2   | CMQ  | G     | 507  | 31/31 | 0.92 | 0.09 | 32,41,56,57                 | 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.



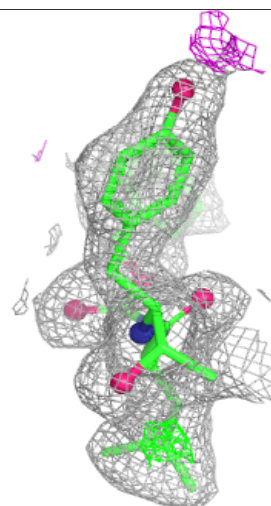
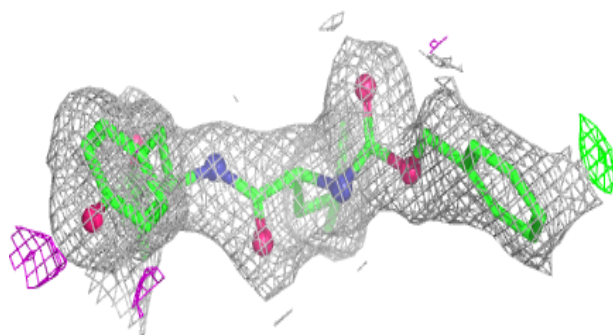
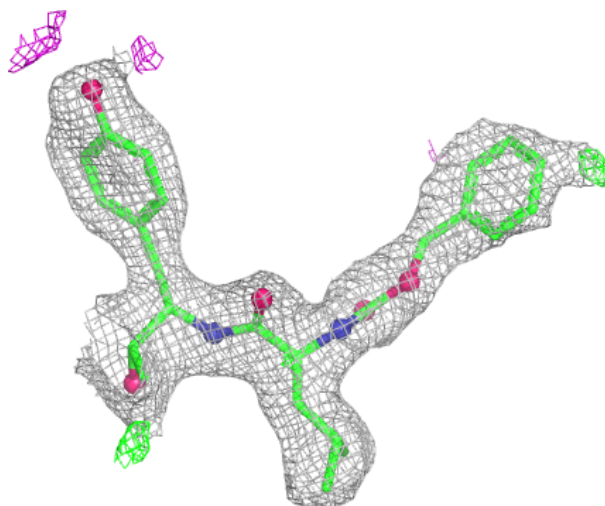
**Electron density around CMQ I 509:**

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



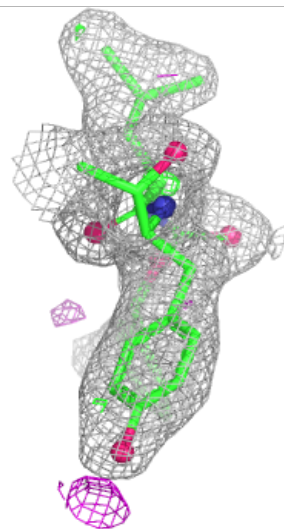
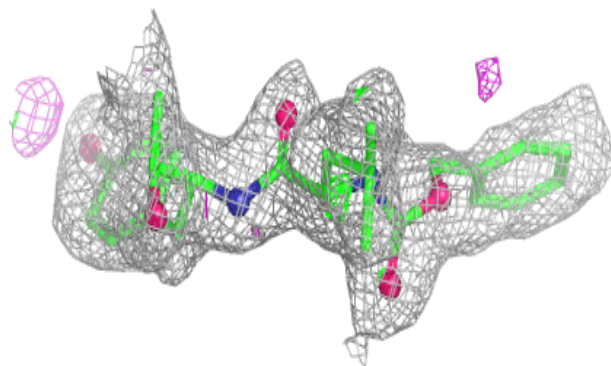
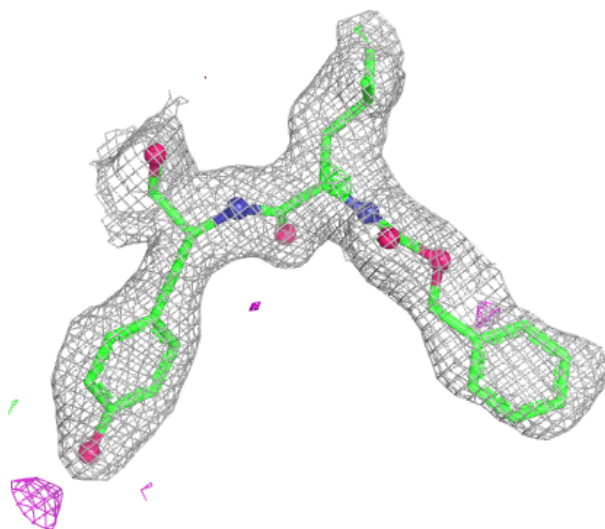
**Electron density around CMQ K 511:**

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



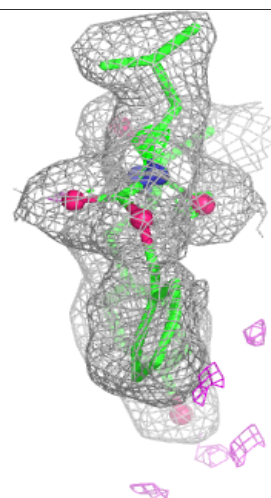
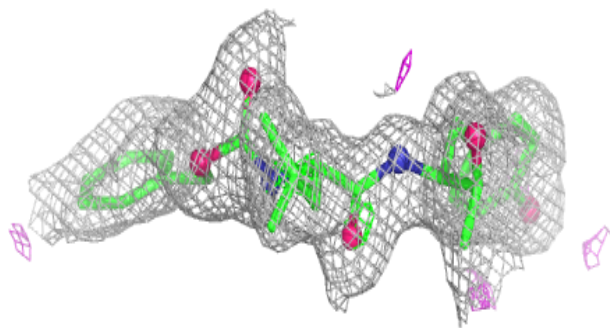
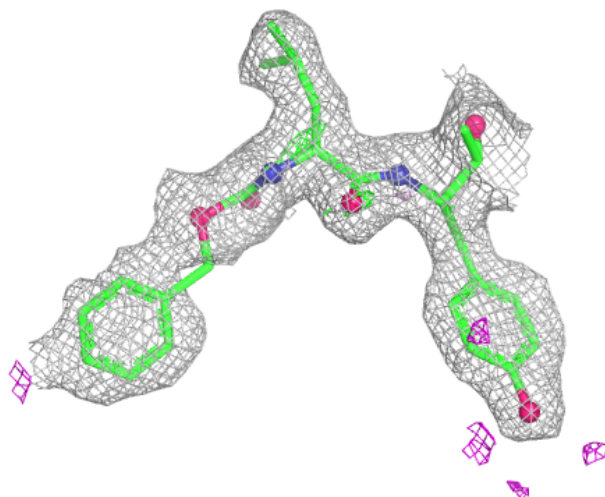
**Electron density around CMQ N 514:**

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



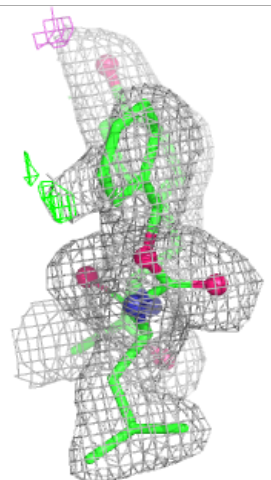
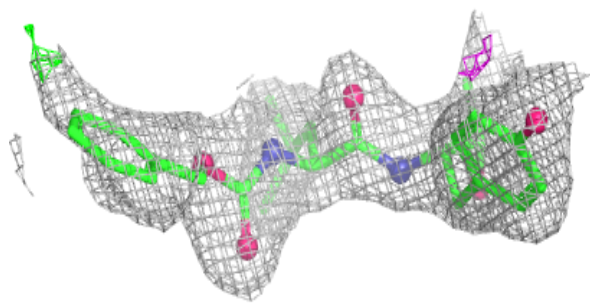
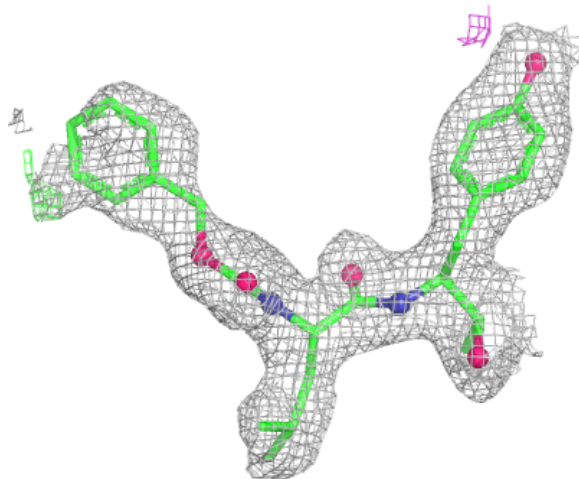
**Electron density around CMQ E 505:**

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



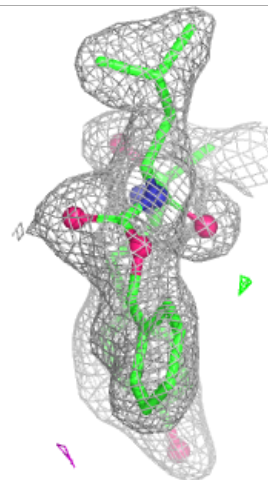
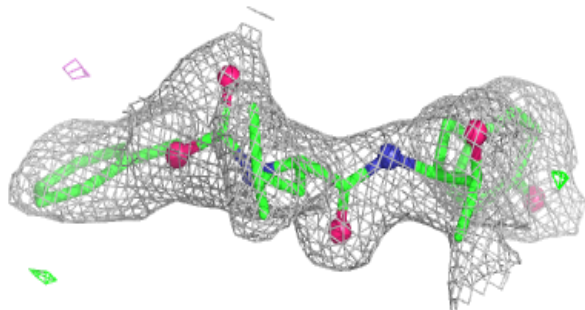
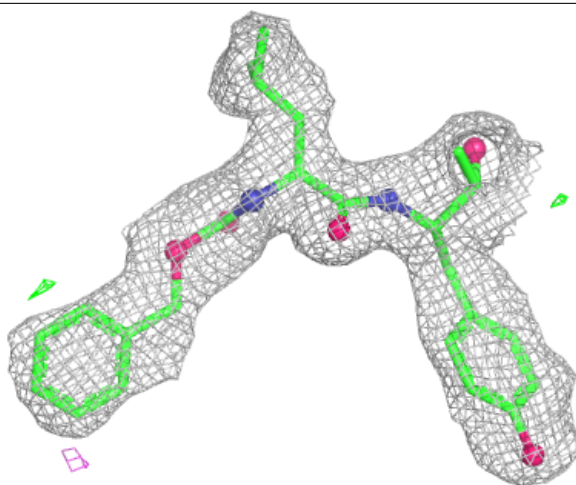
**Electron density around CMQ H 508:**

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



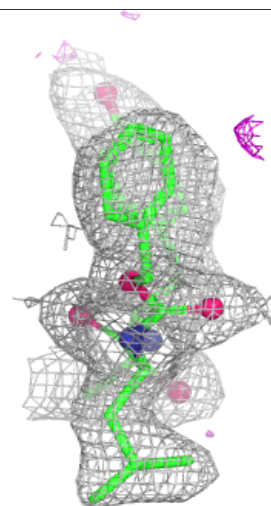
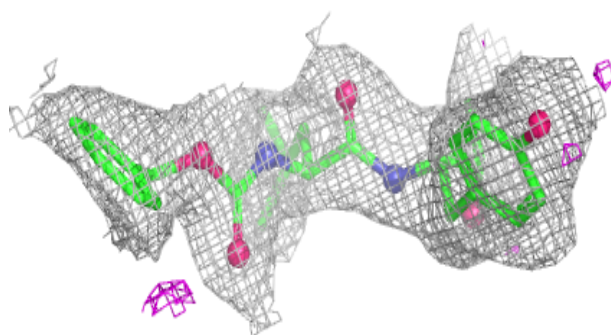
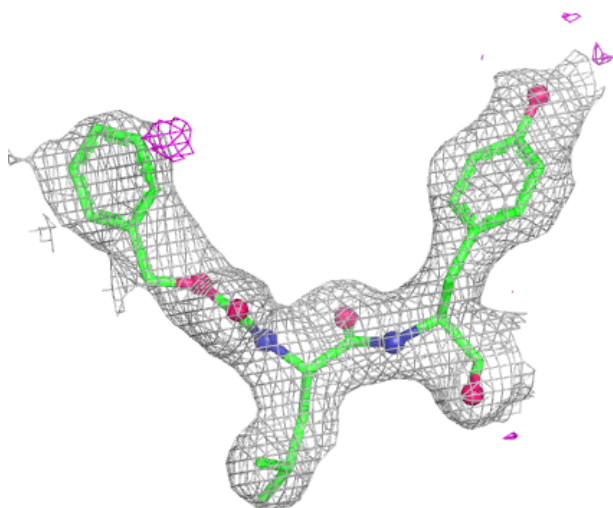
**Electron density around CMQ C 503:**

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



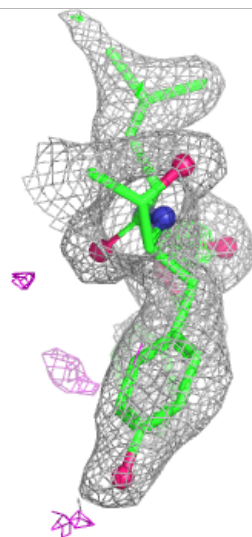
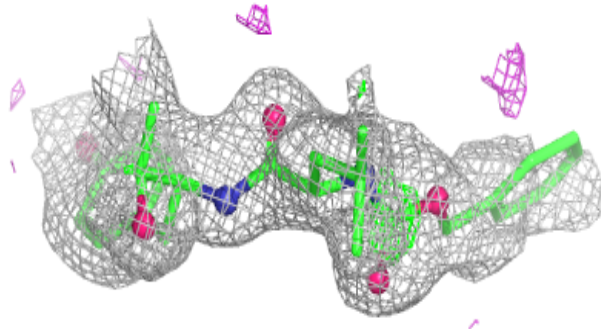
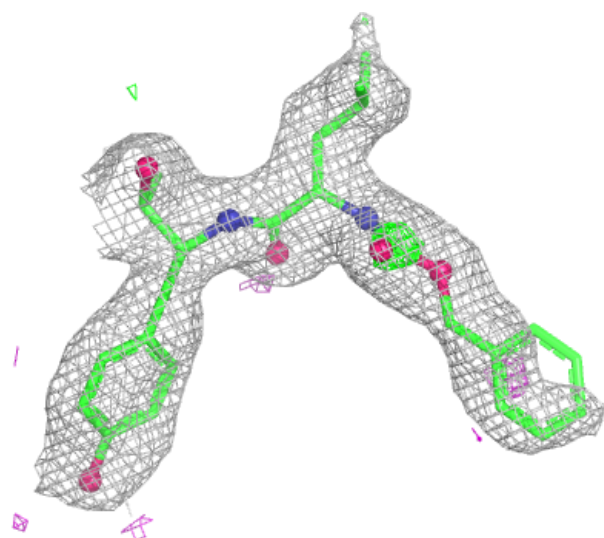
**Electron density around CMQ J 510:**

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



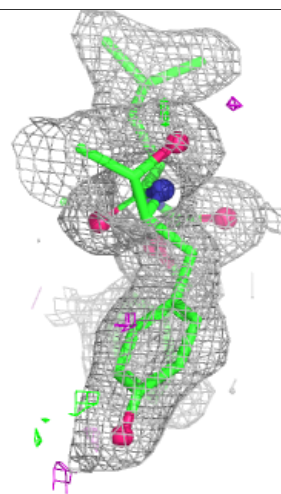
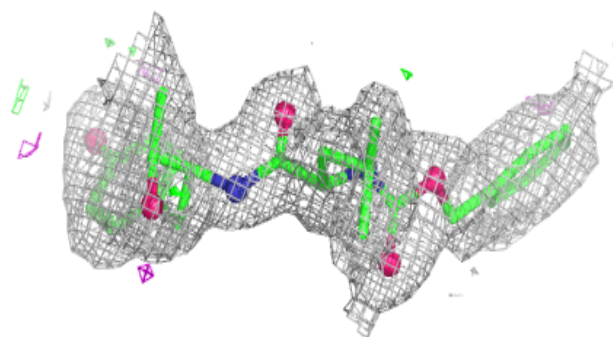
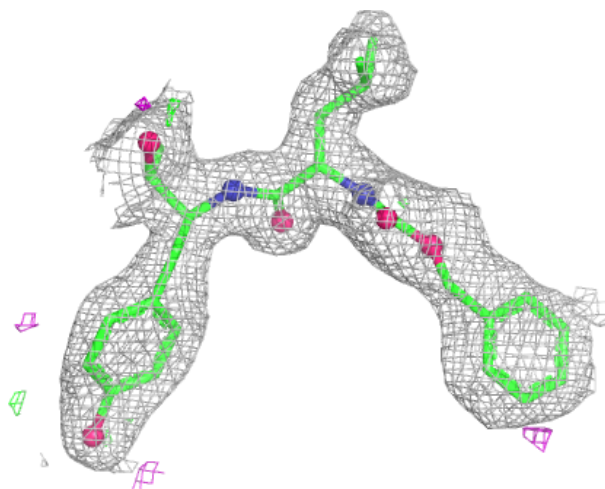
**Electron density around CMQ B 502:**

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



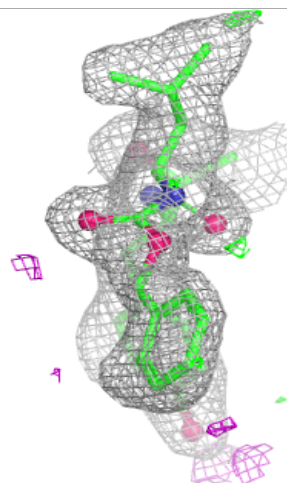
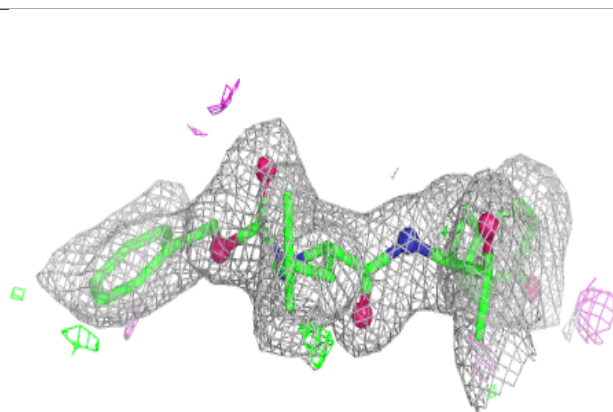
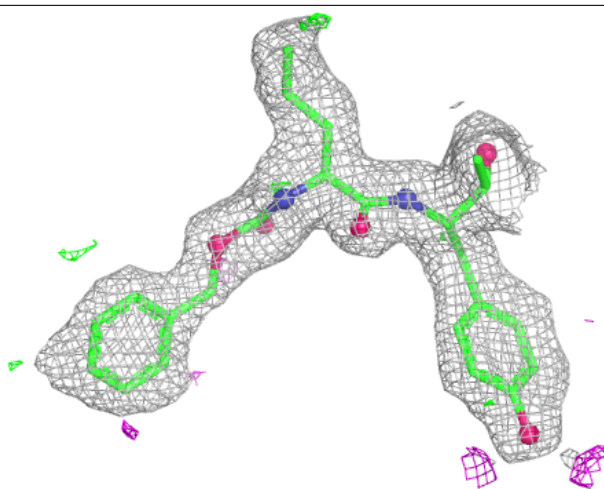
**Electron density around CMQ F 506:**

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



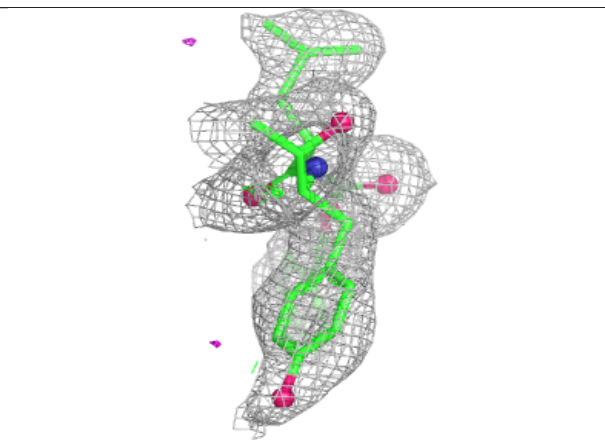
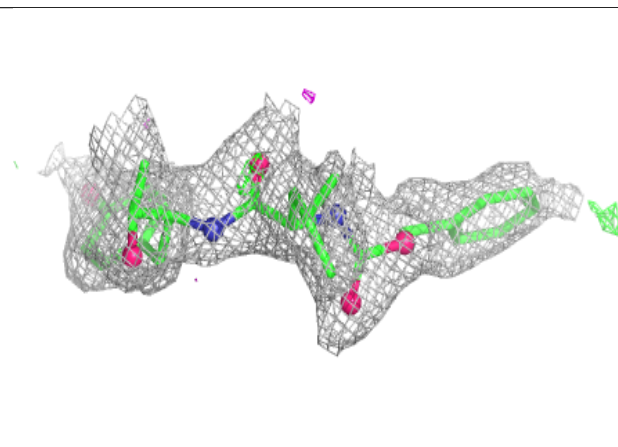
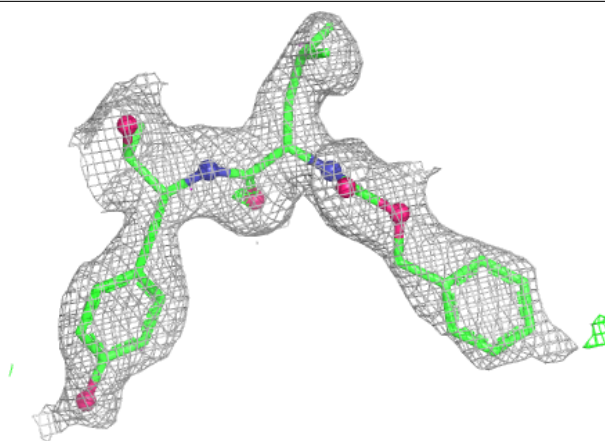
**Electron density around CMQ M 513:**

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



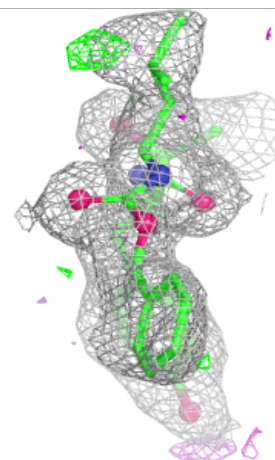
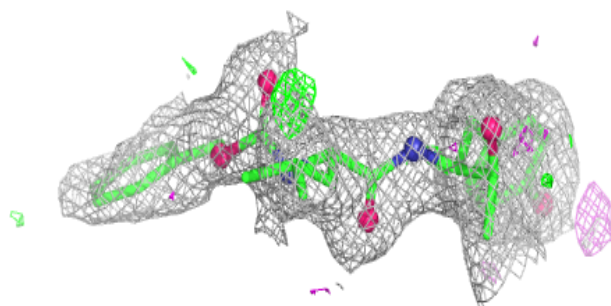
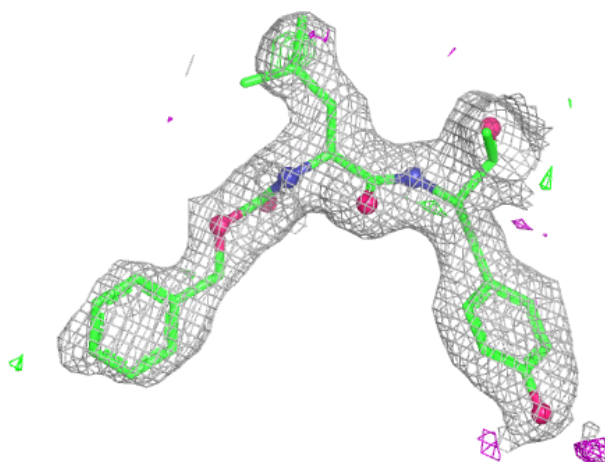
**Electron density around CMQ D 504:**

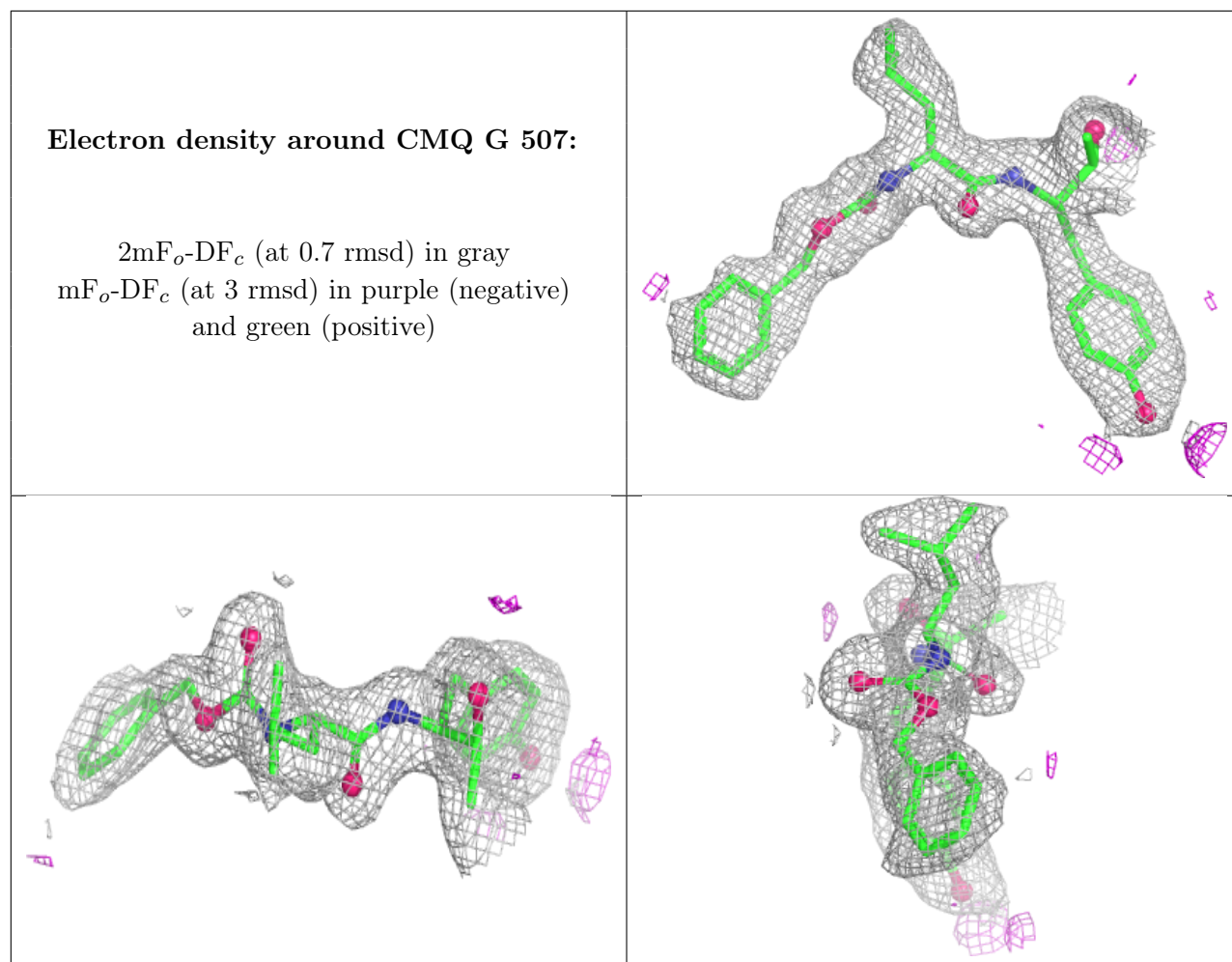
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CMQ L 512:**

$2mF_o-DF_c$  (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.