



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:09 PM EDT

PDB ID : 3T6D / pdb\_00003t6d  
Title : Crystal Structure of the Reaction Centre from Blastochloris viridis strain DSM 133 (ATCC 19567) substrain-08  
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.  
Deposited on : 2011-07-28  
Resolution : 1.95 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                           | : | 9.0.015 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

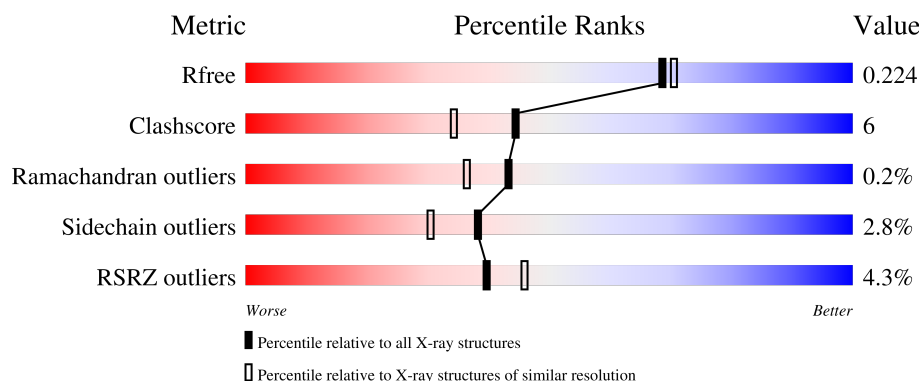
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

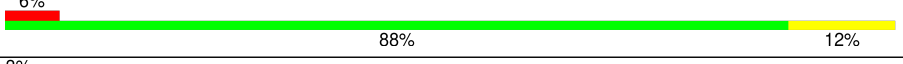
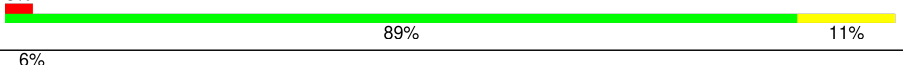
The reported resolution of this entry is 1.95 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3494 (1.96-1.96)                                      |
| Clashscore            | 190562                      | 3612 (1.96-1.96)                                      |
| Ramachandran outliers | 187476                      | 3587 (1.96-1.96)                                      |
| Sidechain outliers    | 187428                      | 3587 (1.96-1.96)                                      |
| RSRZ outliers         | 180081                      | 3495 (1.96-1.96)                                      |

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   | C     | 356    |  |
| 2   | H     | 258    |  |
| 3   | L     | 273    |  |
| 4   | M     | 323    |  |

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 |
|-----|------|-------|--------|-----------|----------|---------|------------------|
| 10  | GOL  | C     | 370    | -         | -        | -       | X                |
| 10  | GOL  | C     | 373    | -         | -        | -       | X                |
| 10  | GOL  | C     | 377    | -         | -        | X       | -                |
| 11  | BCB  | L     | 400    | X         | -        | -       | -                |
| 11  | BCB  | L     | 401    | X         | -        | -       | -                |
| 11  | BCB  | M     | 400    | X         | -        | -       | -                |
| 11  | BCB  | M     | 401    | X         | -        | -       | -                |
| 17  | HTH  | M     | 332    | -         | -        | -       | X                |
| 5   | HEC  | C     | 401    | X         | -        | -       | -                |
| 5   | HEC  | C     | 402    | X         | -        | -       | -                |
| 5   | HEC  | C     | 403    | X         | -        | -       | -                |
| 5   | HEC  | C     | 404    | X         | -        | -       | -                |
| 6   | LDA  | H     | 718[B] | -         | -        | -       | X                |
| 6   | LDA  | L     | 712    | -         | -        | -       | X                |
| 8   | SO4  | M     | 326    | -         | -        | X       | -                |
| 9   | HTO  | C     | 355    | -         | -        | X       | -                |
| 9   | HTO  | C     | 358[A] | -         | X        | -       | -                |
| 9   | HTO  | H     | 274[A] | -         | -        | -       | X                |
| 9   | HTO  | L     | 279    | -         | -        | -       | X                |

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 12156 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 Photosynthetic reaction center cytochrome c subunit.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | C     | 334      | Total | C    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 2647  | 1667 | 474 | 486 | 20 |         |         |       |

- Molecule 2 is a protein called Photosynthetic reaction center H-subunit.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | H     | 258      | Total | C    | N   | O   | S | 44      | 4       | 0     |
|     |       |          | 2035  | 1300 | 353 | 379 | 3 |         |         |       |

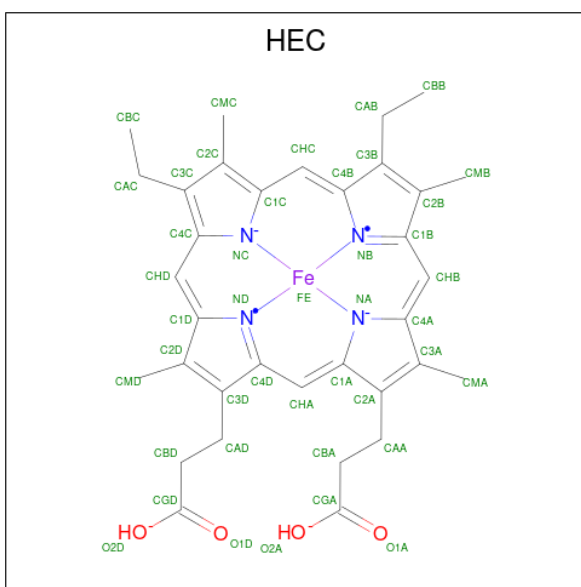
- Molecule 3 is a protein called Photosynthetic reaction center L-subunit.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | L     | 273      | Total | C    | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 2191  | 1474 | 352 | 358 | 7 |         |         |       |

- Molecule 4 is a protein called Photosynthetic reaction center M-subunit.

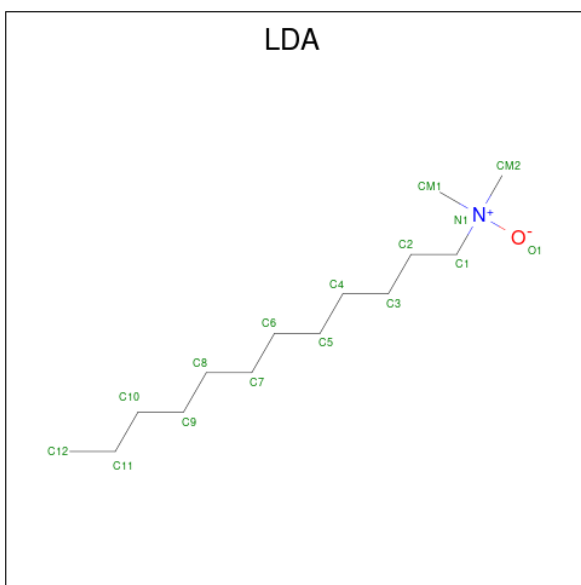
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | M     | 323      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 2574  | 1716 | 424 | 423 | 11 |         |         |       |

- Molecule 5 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{36}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 5   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula:  $\text{C}_{14}\text{H}_{31}\text{NO}$ ).



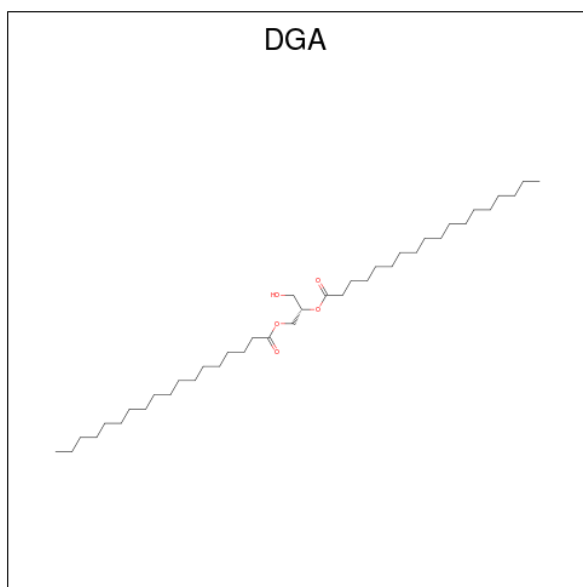
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 6   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | H     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | H     | 1        | Total | C  | N | O | 0       | 1       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | H     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | H     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | H     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 6   | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 6   | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |

- Molecule 7 is DIACYL GLYCEROL (CCD ID: DGA) (formula:  $C_{39}H_{76}O_5$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 7   | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 33 | 4 |         |         |

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula:  $O_4S$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 8   | C     | 1        | Total | O | S | 0       | 1       |
|     |       |          | 10    | 8 | 2 |         |         |
| 8   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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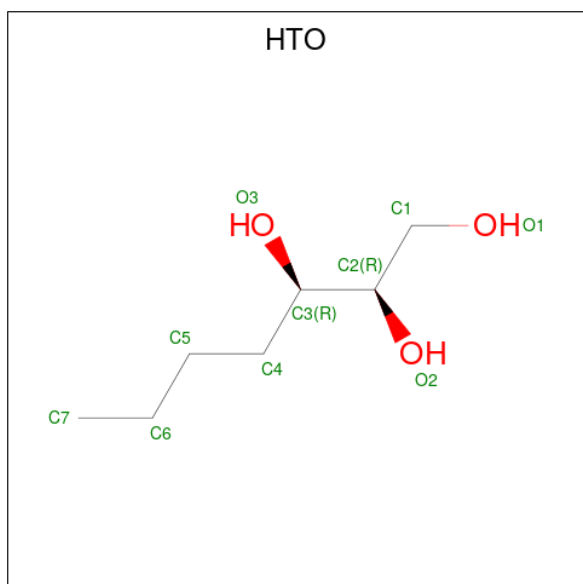
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 8   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | H     | 1        | Total | O | S | 0       | 1       |
|     |       |          | 10    | 8 | 2 |         |         |
| 8   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | L     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | L     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 8   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 8   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 9 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).



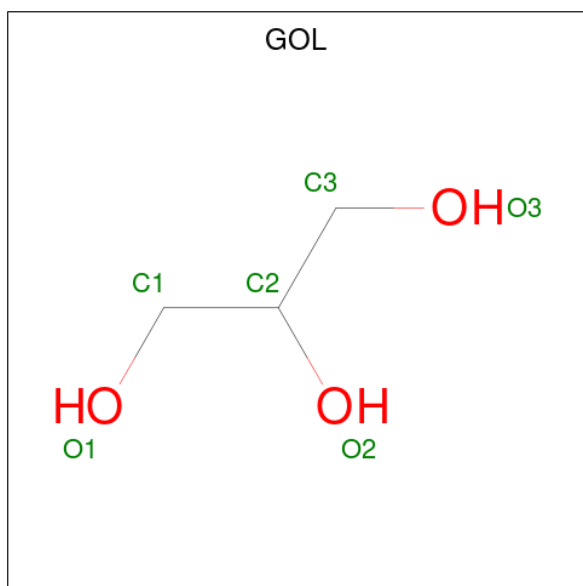
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 9   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 7 | 3 |         |         |
| 9   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 7 | 3 |         |         |
| 9   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 7 | 3 |         |         |
| 9   | C     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 10    | 7 | 3 |         |         |
| 9   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 7 | 3 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 9   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 7 | 3 |         |         |
| 9   | H     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 10    | 7 | 3 |         |         |
| 9   | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 7 | 3 |         |         |
| 9   | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 7 | 3 |         |         |
| 9   | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 7 | 3 |         |         |
| 9   | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 7 | 3 |         |         |
| 9   | M     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 7 | 3 |         |         |

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

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| Mol | Chain | Residues | Atoms      |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 10  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 10  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 10  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 10  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 10  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 10  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 10  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 10  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 10  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 10  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 10  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 10  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 10  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 1       |
| 10  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 10  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 10  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 10  | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 10  | H     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 10  | H     | 1        | Total<br>8 | C<br>4 | O<br>4 | 0       | 1       |
| 10  | H     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 10  | H     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |

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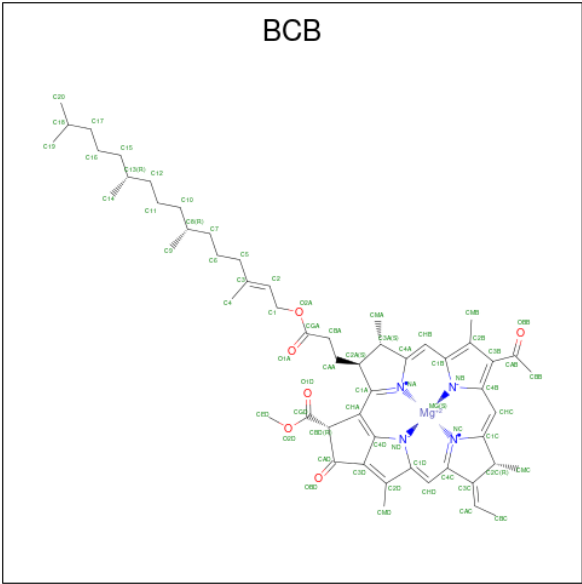
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 10  | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 10  | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 10  | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 10  | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 10  | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 10  | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 10  | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 10  | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 10  | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 10  | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 10  | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 10  | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 10  | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 10  | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 10  | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 10  | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

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

- Molecule 11 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>6</sub>).



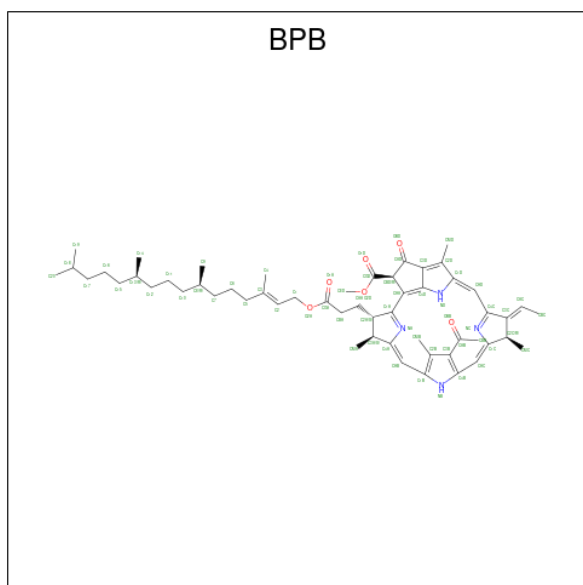
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 11  | L     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |         |
| 11  | L     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |         |

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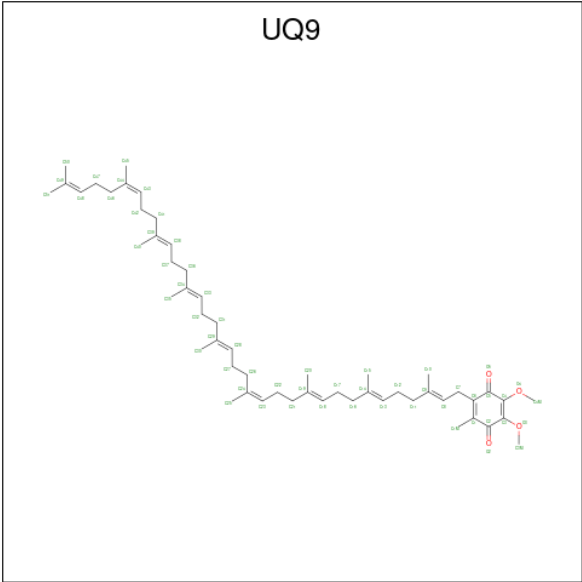
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 11  | M     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |         |
| 11  | M     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |         |

- Molecule 12 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula:  $C_{55}H_{74}N_4O_6$ ).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 12  | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 4 | 6 |         |         |
| 12  | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 4 | 6 |         |         |

- Molecule 13 is Ubiquinone-9 (CCD ID: UQ9) (formula:  $C_{54}H_{82}O_4$ ).

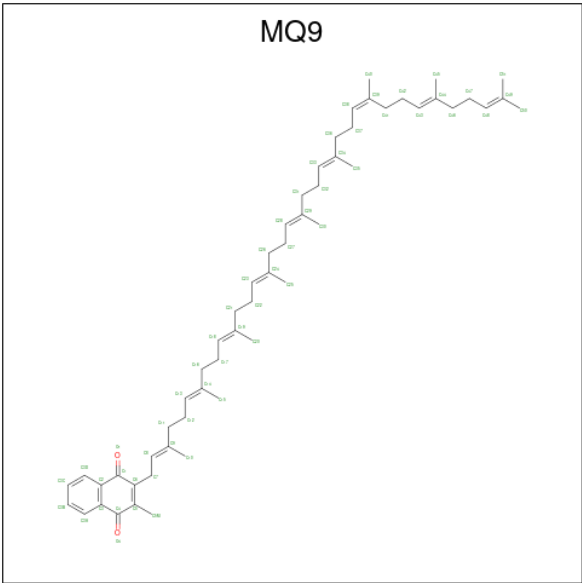


| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 13  | L     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 58    | 54 | 4 |         |         |
| 13  | L     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 23    | 19 | 4 |         |         |

- Molecule 14 is FE (II) ION (CCD ID: FE2) (formula: Fe).

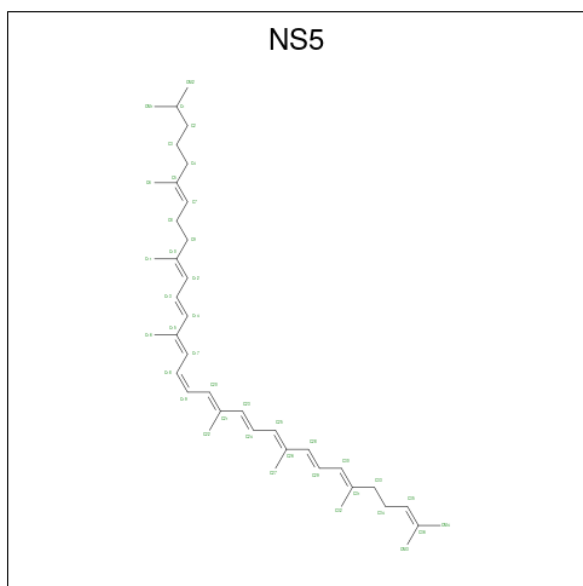
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 14  | M     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 15 is MENAQUINONE-9 (CCD ID: MQ9) (formula: C<sub>56</sub>H<sub>80</sub>O<sub>2</sub>).



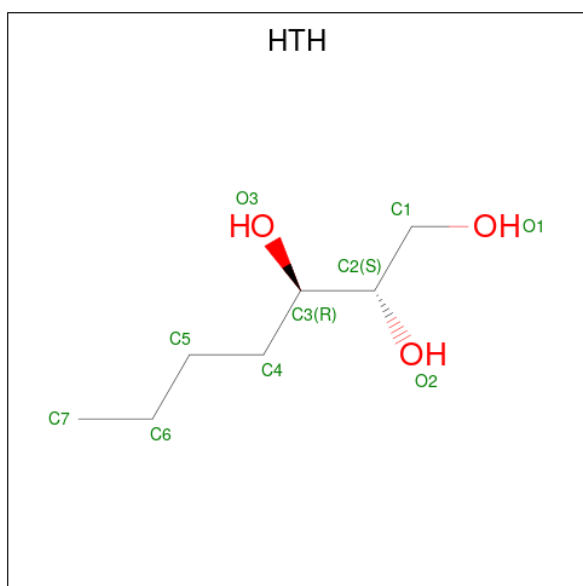
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 15  | M     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 58    | 56 | 2 |         |         |

- Molecule 16 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: C<sub>40</sub>H<sub>60</sub>).



| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 16  | M     | 1        | Total | C  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |

- Molecule 17 is (2S,3R)-heptane-1,2,3-triol (CCD ID: HTH) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 17  | M     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 7 | 3 |         |         |

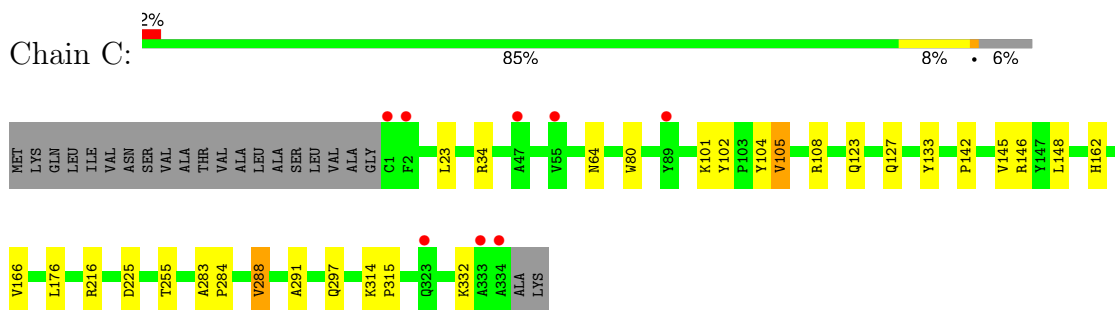
- Molecule 18 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 18  | C     | 388      | Total | O   | 0       | 0       |
|     |       |          | 388   | 388 |         |         |
| 18  | H     | 211      | Total | O   | 0       | 0       |
|     |       |          | 211   | 211 |         |         |
| 18  | L     | 109      | Total | O   | 0       | 0       |
|     |       |          | 109   | 109 |         |         |
| 18  | M     | 153      | Total | O   | 0       | 0       |
|     |       |          | 153   | 153 |         |         |

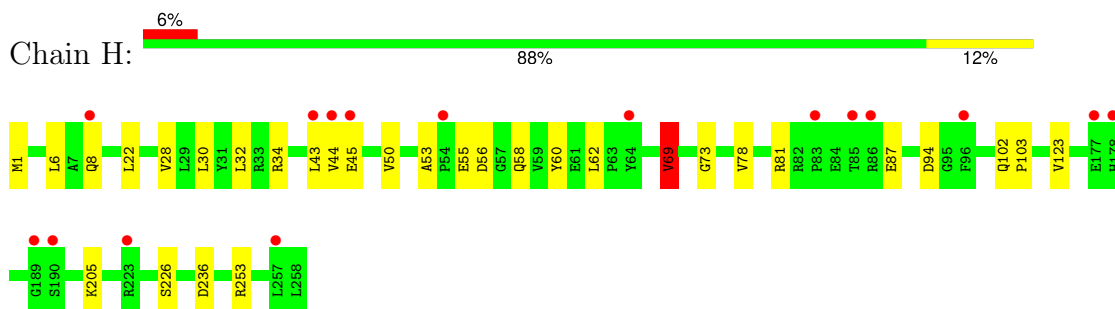
### 3 Residue-property plots [i](#)

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

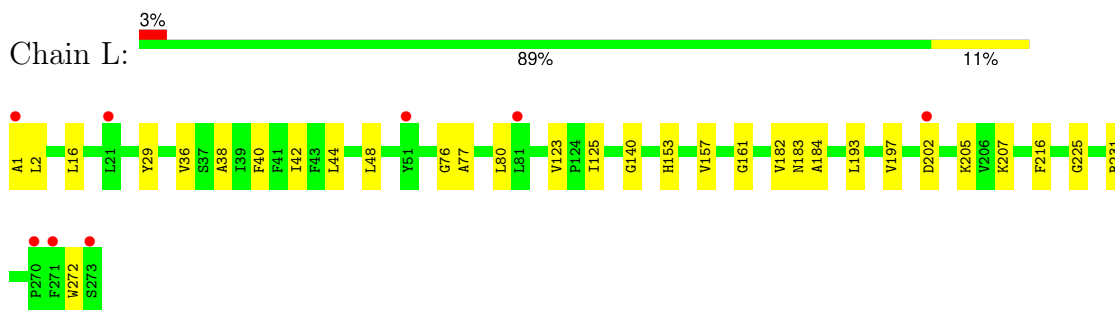
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



- Molecule 2: Photosynthetic reaction center H-subunit

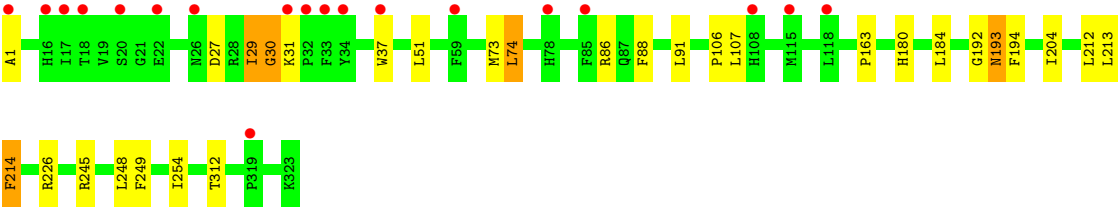


- Molecule 3: Photosynthetic reaction center L-subunit



- Molecule 4: Photosynthetic reaction center M-subunit





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 43 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 220.44Å 220.44Å 113.10Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 48.34 – 1.95<br>48.34 – 1.95                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.2 (48.34-1.95)<br>96.2 (48.34-1.95)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.09                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.06 (at 1.95Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.6.0101                                             | Depositor        |
| R, $R_{free}$                                                           | 0.182 , 0.216<br>0.193 , 0.224                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 9677 reflections (5.01%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 39.5                                                        | Xtriage          |
| Anisotropy                                                              | 0.113                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 92.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 12156                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 51.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: BCB, HTH, HTO, LDA, BPB, NS5, FE2, GOL, DGA, SO4, FME, UQ9, MQ9, HEC

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   | C     | 1.11         | 1/2716 (0.0%) | 1.01        | 3/3701 (0.1%)   |
| 2   | H     | 1.12         | 3/2069 (0.1%) | 0.98        | 6/2827 (0.2%)   |
| 3   | L     | 1.14         | 3/2280 (0.1%) | 0.98        | 2/3113 (0.1%)   |
| 4   | M     | 1.17         | 2/2679 (0.1%) | 1.01        | 4/3662 (0.1%)   |
| All | All   | 1.14         | 9/9744 (0.1%) | 1.00        | 15/13303 (0.1%) |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 142 | PRO  | CA-C  | 6.86  | 1.55        | 1.51     |
| 2   | H     | 53  | ALA  | CA-C  | -6.55 | 1.44        | 1.52     |
| 2   | H     | 78  | VAL  | C-O   | 5.66  | 1.28        | 1.24     |
| 2   | H     | 73  | GLY  | C-O   | -5.61 | 1.17        | 1.24     |
| 4   | M     | 312 | THR  | C-O   | -5.58 | 1.20        | 1.25     |
| 4   | M     | 245 | ARG  | C-O   | -5.58 | 1.17        | 1.24     |
| 3   | L     | 184 | ALA  | CA-CB | 5.47  | 1.61        | 1.53     |
| 3   | L     | 40  | PHE  | N-CA  | -5.37 | 1.40        | 1.46     |
| 3   | L     | 123 | VAL  | CA-CB | -5.12 | 1.51        | 1.54     |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 288 | VAL  | CB-CA-C | -7.46 | 104.14      | 111.30   |
| 2   | H     | 69  | VAL  | CB-CA-C | 7.34  | 119.84      | 110.96   |
| 1   | C     | 102 | TYR  | CA-C-N  | -6.33 | 113.17      | 119.56   |
| 1   | C     | 102 | TYR  | C-N-CA  | -6.33 | 113.17      | 119.56   |
| 4   | M     | 30  | GLY  | N-CA-C  | -6.29 | 105.25      | 112.29   |
| 2   | H     | 53  | ALA  | O-C-N   | -6.06 | 114.35      | 121.32   |
| 2   | H     | 32  | LEU  | N-CA-C  | 5.97  | 117.45      | 111.07   |
| 3   | L     | 225 | GLY  | CA-C-N  | 5.65  | 127.79      | 120.44   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | L     | 225 | GLY  | C-N-CA | 5.65  | 127.79      | 120.44   |
| 4   | M     | 254 | ILE  | N-CA-C | 5.58  | 118.36      | 112.83   |
| 2   | H     | 28  | VAL  | N-CA-C | 5.44  | 115.64      | 110.42   |
| 4   | M     | 204 | ILE  | N-CA-C | 5.39  | 116.12      | 110.62   |
| 2   | H     | 45  | GLU  | CA-C-N | -5.18 | 113.20      | 118.85   |
| 2   | H     | 45  | GLU  | C-N-CA | -5.18 | 113.20      | 118.85   |
| 4   | M     | 31  | LYS  | N-CA-C | -5.08 | 101.72      | 109.64   |

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   | C     | 2647  | 0        | 2610     | 30      | 0            |
| 2   | H     | 2035  | 0        | 2017     | 14      | 0            |
| 3   | L     | 2191  | 0        | 2116     | 22      | 0            |
| 4   | M     | 2574  | 0        | 2470     | 31      | 0            |
| 5   | C     | 172   | 0        | 120      | 1       | 0            |
| 6   | C     | 32    | 0        | 62       | 3       | 0            |
| 6   | H     | 80    | 0        | 155      | 1       | 0            |
| 6   | L     | 144   | 0        | 279      | 8       | 0            |
| 6   | M     | 128   | 0        | 248      | 11      | 0            |
| 7   | C     | 37    | 0        | 58       | 3       | 0            |
| 8   | C     | 95    | 0        | 0        | 1       | 0            |
| 8   | H     | 70    | 0        | 0        | 0       | 0            |
| 8   | L     | 10    | 0        | 0        | 0       | 0            |
| 8   | M     | 40    | 0        | 0        | 2       | 0            |
| 9   | C     | 40    | 0        | 64       | 8       | 0            |
| 9   | H     | 30    | 0        | 48       | 4       | 0            |
| 9   | L     | 50    | 0        | 80       | 3       | 0            |
| 9   | M     | 10    | 0        | 16       | 0       | 0            |
| 10  | C     | 120   | 0        | 160      | 13      | 0            |
| 10  | H     | 104   | 0        | 135      | 4       | 0            |
| 10  | L     | 48    | 0        | 64       | 1       | 0            |
| 10  | M     | 54    | 0        | 72       | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11  | L     | 132   | 0        | 144      | 9       | 0            |
| 11  | M     | 132   | 0        | 144      | 17      | 0            |
| 12  | L     | 65    | 0        | 74       | 0       | 0            |
| 12  | M     | 65    | 0        | 74       | 0       | 0            |
| 13  | L     | 81    | 0        | 105      | 16      | 0            |
| 14  | M     | 1     | 0        | 0        | 0       | 0            |
| 15  | M     | 58    | 0        | 80       | 2       | 0            |
| 16  | M     | 40    | 0        | 60       | 3       | 0            |
| 17  | M     | 10    | 0        | 16       | 0       | 0            |
| 18  | C     | 388   | 0        | 0        | 2       | 0            |
| 18  | H     | 211   | 0        | 0        | 2       | 0            |
| 18  | L     | 109   | 0        | 0        | 0       | 0            |
| 18  | M     | 153   | 0        | 0        | 0       | 0            |
| All | All   | 12156 | 0        | 11471    | 137     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (137) 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) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:L:502:UQ9:H15A  | 11:M:400:BCB:C9   | 1.75                     | 1.15              |
| 13:L:502:UQ9:H15A  | 11:M:400:BCB:H93  | 1.46                     | 0.98              |
| 13:L:502:UQ9:H15A  | 11:M:400:BCB:H91  | 1.49                     | 0.94              |
| 6:C:716:LDA:H51    | 10:H:280:GOL:O1   | 1.75                     | 0.85              |
| 3:L:272:TRP:CD1    | 4:M:86:ARG:HD3    | 2.13                     | 0.83              |
| 4:M:73:MET:HE1     | 4:M:88:PHE:CE1    | 2.16                     | 0.80              |
| 4:M:29:ILE:CD1     | 4:M:51:LEU:HD13   | 2.14                     | 0.77              |
| 10:C:364:GOL:H11   | 6:M:715:LDA:HM11  | 1.68                     | 0.76              |
| 1:C:34:ARG:HD3     | 9:C:357:HTO:H3    | 1.65                     | 0.75              |
| 4:M:29:ILE:HD11    | 4:M:51:LEU:HD13   | 1.70                     | 0.74              |
| 1:C:297:GLN:HE22   | 10:C:365:GOL:H31  | 1.53                     | 0.73              |
| 11:M:400:BCB:HBB2  | 11:M:400:BCB:HMB3 | 1.68                     | 0.73              |
| 1:C:255:THR:HG23   | 10:C:363:GOL:H32  | 1.72                     | 0.72              |
| 1:C:64[A]:ASN:HD21 | 9:C:355:HTO:C2    | 2.03                     | 0.71              |
| 2:H:226:SER:HB3    | 9:H:272:HTO:H42   | 1.72                     | 0.71              |
| 4:M:73:MET:HE1     | 4:M:88:PHE:CD1    | 2.30                     | 0.67              |
| 11:L:400:BCB:HMB1  | 11:L:400:BCB:HBB3 | 1.78                     | 0.66              |
| 1:C:148:LEU:HD13   | 10:C:365:GOL:H12  | 1.78                     | 0.66              |
| 13:L:502:UQ9:C15   | 11:M:400:BCB:H91  | 2.26                     | 0.65              |
| 4:M:29:ILE:HD12    | 4:M:51:LEU:HD22   | 1.78                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:L:231:ARG:HG2   | 6:L:723:LDA:HM23   | 1.80                     | 0.63              |
| 1:C:332:LYS:H     | 9:C:355:HTO:H71    | 1.63                     | 0.63              |
| 10:C:364:GOL:C1   | 6:M:715:LDA:HM11   | 2.30                     | 0.62              |
| 2:H:253:ARG:HE    | 10:H:278:GOL:H31   | 1.64                     | 0.62              |
| 1:C:291:ALA:HB3   | 10:C:377:GOL:C3    | 2.29                     | 0.62              |
| 13:L:503:UQ9:O5   | 13:L:503:UQ9:H4MA  | 2.01                     | 0.61              |
| 13:L:502:UQ9:C15  | 11:M:400:BCB:H93   | 2.27                     | 0.61              |
| 4:M:73:MET:HE3    | 4:M:91:LEU:HB2     | 1.83                     | 0.61              |
| 6:L:710:LDA:H32   | 9:L:277:HTO:H73    | 1.83                     | 0.59              |
| 2:H:253:ARG:HE    | 10:H:278:GOL:C3    | 2.16                     | 0.59              |
| 13:L:503:UQ9:O5   | 13:L:503:UQ9:H8    | 2.03                     | 0.59              |
| 4:M:30:GLY:HA3    | 10:M:342:GOL:H12   | 1.85                     | 0.58              |
| 3:L:36:VAL:HG12   | 9:L:279:HTO:H3     | 1.85                     | 0.58              |
| 11:L:401:BCB:HMB1 | 11:L:401:BCB:CBB   | 2.34                     | 0.57              |
| 1:C:291:ALA:HB3   | 10:C:377:GOL:H31   | 1.86                     | 0.57              |
| 11:L:400:BCB:H193 | 15:M:501:MQ9:H252  | 1.87                     | 0.57              |
| 4:M:74:LEU:CD1    | 16:M:600:NS5:HM23  | 2.36                     | 0.56              |
| 4:M:1:ALA:N       | 8:M:326:SO4:O3     | 2.31                     | 0.56              |
| 8:C:338:SO4:O4    | 10:M:334:GOL:O1    | 2.21                     | 0.56              |
| 2:H:205:LYS:O     | 10:H:279:GOL:O1    | 2.23                     | 0.55              |
| 1:C:101:LYS:NZ    | 18:C:631:HOH:O     | 2.40                     | 0.55              |
| 4:M:212:LEU:C     | 4:M:212:LEU:HD23   | 2.32                     | 0.55              |
| 3:L:140:GLY:HA3   | 6:L:712:LDA:HM13   | 1.88                     | 0.55              |
| 3:L:38:ALA:O      | 3:L:42:ILE:HG13    | 2.07                     | 0.54              |
| 4:M:37:TRP:HD1    | 6:M:704:LDA:CM1    | 2.21                     | 0.54              |
| 1:C:123:GLN:HE21  | 10:M:338:GOL:H11   | 1.72                     | 0.54              |
| 2:H:81[A]:ARG:HG3 | 2:H:81[A]:ARG:HH11 | 1.72                     | 0.54              |
| 3:L:76:GLY:HA3    | 6:L:711:LDA:HM13   | 1.89                     | 0.54              |
| 4:M:37:TRP:CD1    | 6:M:704:LDA:HM12   | 2.44                     | 0.53              |
| 2:H:6:LEU:HD23    | 9:H:274[A]:HTO:H2  | 1.90                     | 0.53              |
| 7:C:730:DGA:HB22  | 7:C:730:DGA:HA22   | 1.91                     | 0.53              |
| 2:H:43:LEU:HB3    | 3:L:1:ALA:HB1      | 1.90                     | 0.53              |
| 13:L:502:UQ9:C15  | 11:M:400:BCB:C9    | 2.67                     | 0.53              |
| 1:C:123:GLN:HE21  | 10:M:338:GOL:H31   | 1.74                     | 0.52              |
| 2:H:62:LEU:O      | 6:H:721:LDA:HM21   | 2.08                     | 0.52              |
| 1:C:162:HIS:HB2   | 10:C:368:GOL:H2    | 1.92                     | 0.52              |
| 1:C:291:ALA:N     | 10:C:377:GOL:H32   | 2.25                     | 0.52              |
| 3:L:193:LEU:HD22  | 3:L:216:PHE:CE2    | 2.44                     | 0.52              |
| 3:L:272:TRP:CG    | 4:M:86:ARG:HD3     | 2.45                     | 0.52              |
| 4:M:37:TRP:HD1    | 6:M:704:LDA:HM12   | 1.75                     | 0.51              |
| 1:C:283:ALA:HB3   | 1:C:284:PRO:HD3    | 1.92                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:M:400:BCB:HBB2  | 11:M:400:BCB:CMB  | 2.39                     | 0.51              |
| 1:C:314:LYS:HZ2    | 10:C:373:GOL:H2   | 1.75                     | 0.51              |
| 1:C:225:ASP:OD1    | 10:C:369:GOL:O3   | 2.29                     | 0.51              |
| 3:L:231:ARG:CG     | 6:L:723:LDA:HM23  | 2.40                     | 0.50              |
| 11:L:400:BCB:HMB1  | 11:L:400:BCB:CBB  | 2.41                     | 0.50              |
| 11:M:401:BCB:HMB3  | 11:M:401:BCB:CBB  | 2.42                     | 0.50              |
| 13:L:503:UQ9:H3MB  | 13:L:503:UQ9:O4   | 2.11                     | 0.50              |
| 4:M:37:TRP:H       | 6:M:704:LDA:HM13  | 1.77                     | 0.50              |
| 1:C:145:VAL:O      | 1:C:146:ARG:HD2   | 2.11                     | 0.50              |
| 11:L:400:BCB:OBB   | 11:L:400:BCB:HHC  | 2.11                     | 0.49              |
| 1:C:291:ALA:HB3    | 10:C:377:GOL:H32  | 1.95                     | 0.49              |
| 9:H:273:HTO:C1     | 18:H:499:HOH:O    | 2.60                     | 0.49              |
| 1:C:64[A]:ASN:ND2  | 9:C:355:HTO:H3    | 2.27                     | 0.49              |
| 3:L:193:LEU:HD22   | 3:L:216:PHE:HE2   | 1.77                     | 0.49              |
| 13:L:503:UQ9:O5    | 13:L:503:UQ9:C8   | 2.60                     | 0.49              |
| 13:L:502:UQ9:O2    | 13:L:502:UQ9:H3MB | 2.13                     | 0.49              |
| 4:M:192:GLY:O      | 4:M:193:ASN:HB3   | 2.13                     | 0.49              |
| 1:C:105:VAL:CG2    | 1:C:288:VAL:HG11  | 2.43                     | 0.48              |
| 9:H:273:HTO:H12    | 18:H:499:HOH:O    | 2.12                     | 0.48              |
| 7:C:730:DGA:HB62   | 7:C:730:DGA:HA52  | 1.94                     | 0.48              |
| 2:H:69:VAL:HG22    | 3:L:205:LYS:HA    | 1.94                     | 0.47              |
| 1:C:64[A]:ASN:HD21 | 9:C:355:HTO:C3    | 2.27                     | 0.47              |
| 1:C:123:GLN:NE2    | 10:M:338:GOL:H31  | 2.29                     | 0.47              |
| 11:L:401:BCB:HMB1  | 11:L:401:BCB:HBB2 | 1.96                     | 0.47              |
| 4:M:73:MET:HE1     | 4:M:88:PHE:HE1    | 1.75                     | 0.47              |
| 3:L:161:GLY:HA3    | 11:L:400:BCB:HAC1 | 1.96                     | 0.47              |
| 4:M:29:ILE:HD12    | 4:M:51:LEU:HD13   | 1.96                     | 0.46              |
| 4:M:74:LEU:HD12    | 16:M:600:NS5:CM2  | 2.45                     | 0.46              |
| 4:M:226:ARG:NH1    | 8:M:326:SO4:O1    | 2.44                     | 0.46              |
| 3:L:272:TRP:CD1    | 4:M:86:ARG:CD     | 2.93                     | 0.46              |
| 1:C:108:ARG:HD2    | 18:C:780:HOH:O    | 2.15                     | 0.46              |
| 3:L:125:ILE:HG21   | 6:L:724:LDA:HM22  | 1.97                     | 0.46              |
| 4:M:106:PRO:HB3    | 6:M:714:LDA:H31   | 1.98                     | 0.46              |
| 1:C:64[A]:ASN:HD21 | 9:C:355:HTO:H3    | 1.80                     | 0.46              |
| 4:M:184:LEU:HD21   | 11:M:400:BCB:CAC  | 2.47                     | 0.45              |
| 11:M:401:BCB:HAA2  | 11:M:401:BCB:HBD  | 1.98                     | 0.45              |
| 2:H:81[A]:ARG:HG3  | 2:H:81[A]:ARG:NH1 | 2.32                     | 0.45              |
| 6:C:716:LDA:HM21   | 10:C:364:GOL:O3   | 2.17                     | 0.45              |
| 4:M:107:LEU:H      | 6:M:714:LDA:H32   | 1.82                     | 0.45              |
| 13:L:502:UQ9:H4MB  | 13:L:502:UQ9:O3   | 2.16                     | 0.44              |
| 11:M:401:BCB:HAA2  | 11:M:401:BCB:CBD  | 2.42                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:L:502:UQ9:C51   | 11:M:400:BCB:H191 | 2.47                     | 0.44              |
| 1:C:80:TRP:CD1     | 1:C:133:TYR:HB2   | 2.52                     | 0.44              |
| 7:C:730:DGA:HB22   | 7:C:730:DGA:CA2   | 2.47                     | 0.44              |
| 3:L:182:VAL:HA     | 11:M:400:BCB:H43  | 2.00                     | 0.44              |
| 4:M:74:LEU:HD12    | 16:M:600:NS5:HM23 | 1.99                     | 0.44              |
| 13:L:503:UQ9:O5    | 13:L:503:UQ9:C4M  | 2.65                     | 0.44              |
| 4:M:37:TRP:CD1     | 6:M:704:LDA:CM1   | 3.01                     | 0.43              |
| 2:H:30:LEU:O       | 2:H:34:ARG:HD2    | 2.18                     | 0.43              |
| 3:L:29:TYR:OH      | 6:L:702:LDA:H12   | 2.19                     | 0.43              |
| 3:L:153:HIS:O      | 3:L:157:VAL:HG23  | 2.18                     | 0.43              |
| 4:M:212:LEU:HD23   | 4:M:212:LEU:O     | 2.17                     | 0.43              |
| 3:L:77:ALA:HB1     | 9:L:277:HTO:O3    | 2.18                     | 0.43              |
| 11:M:400:BCB:CMB   | 11:M:400:BCB:CBB  | 2.97                     | 0.43              |
| 2:H:102:GLN:HA     | 2:H:103:PRO:HD3   | 1.94                     | 0.42              |
| 4:M:37:TRP:H       | 6:M:704:LDA:CM1   | 2.32                     | 0.42              |
| 15:M:501:MQ9:C38   | 15:M:501:MQ9:H33  | 2.49                     | 0.42              |
| 11:M:401:BCB:OBB   | 11:M:401:BCB:HHC  | 2.20                     | 0.42              |
| 1:C:104:TYR:C      | 1:C:104:TYR:CD1   | 2.98                     | 0.42              |
| 11:L:401:BCB:OBB   | 11:L:401:BCB:HHC  | 2.20                     | 0.42              |
| 1:C:146:ARG:HD2    | 1:C:146:ARG:HA    | 1.80                     | 0.42              |
| 9:C:357:HTO:H73    | 10:L:286:GOL:O1   | 2.20                     | 0.42              |
| 3:L:125:ILE:CG2    | 6:L:724:LDA:HM22  | 2.51                     | 0.41              |
| 1:C:64[A]:ASN:HD21 | 9:C:355:HTO:C1    | 2.33                     | 0.41              |
| 2:H:55:GLU:H       | 2:H:58:GLN:HE21   | 1.67                     | 0.41              |
| 11:L:401:BCB:O1A   | 11:L:401:BCB:H43  | 2.21                     | 0.41              |
| 1:C:216:ARG:HG3    | 6:C:716:LDA:HM22  | 2.02                     | 0.41              |
| 3:L:197:VAL:HG13   | 3:L:207:LYS:HB2   | 2.02                     | 0.41              |
| 1:C:314:LYS:O      | 1:C:315:PRO:C     | 2.63                     | 0.40              |
| 5:C:401:HEC:HBB3   | 5:C:401:HEC:CMB   | 2.51                     | 0.40              |
| 2:H:56:ASP:HB3     | 2:H:60:TYR:CE2    | 2.56                     | 0.40              |
| 3:L:183:ASN:HD21   | 4:M:214:PHE:HB3   | 1.85                     | 0.40              |
| 13:L:502:UQ9:H32   | 13:L:502:UQ9:H35  | 1.95                     | 0.40              |
| 4:M:248:LEU:O      | 4:M:249:PHE:C     | 2.62                     | 0.40              |
| 6:M:707:LDA:HM13   | 6:M:707:LDA:H21   | 1.81                     | 0.40              |
| 13:L:502:UQ9:H51A  | 11:M:400:BCB:H191 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | C     | 335/356 (94%)   | 326 (97%)  | 9 (3%)  | 0        | 100         | 100 |
| 2   | H     | 259/258 (100%)  | 247 (95%)  | 11 (4%) | 1 (0%)   | 30          | 21  |
| 3   | L     | 273/273 (100%)  | 268 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 4   | M     | 323/323 (100%)  | 315 (98%)  | 7 (2%)  | 1 (0%)   | 36          | 28  |
| All | All   | 1190/1210 (98%) | 1156 (97%) | 32 (3%) | 2 (0%)   | 43          | 36  |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 50  | VAL  |
| 4   | M     | 193 | ASN  |

### 5.3.2 Protein sidechains [i](#)

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   | C     | 286/299 (96%)  | 281 (98%) | 5 (2%)   | 53          | 49 |
| 2   | H     | 209/211 (99%)  | 201 (96%) | 8 (4%)   | 29          | 19 |
| 3   | L     | 220/218 (101%) | 214 (97%) | 6 (3%)   | 39          | 32 |
| 4   | M     | 249/247 (101%) | 241 (97%) | 8 (3%)   | 34          | 25 |
| All | All   | 964/975 (99%)  | 937 (97%) | 27 (3%)  | 38          | 30 |

All (27) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 23  | LEU  |
| 1   | C     | 105 | VAL  |
| 1   | C     | 127 | GLN  |
| 1   | C     | 166 | VAL  |
| 1   | C     | 176 | LEU  |
| 2   | H     | 8   | GLN  |
| 2   | H     | 22  | LEU  |
| 2   | H     | 44  | VAL  |
| 2   | H     | 69  | VAL  |
| 2   | H     | 87  | GLU  |
| 2   | H     | 94  | ASP  |
| 2   | H     | 123 | VAL  |
| 2   | H     | 236 | ASP  |
| 3   | L     | 2   | LEU  |
| 3   | L     | 16  | LEU  |
| 3   | L     | 44  | LEU  |
| 3   | L     | 48  | LEU  |
| 3   | L     | 80  | LEU  |
| 3   | L     | 202 | ASP  |
| 4   | M     | 27  | ASP  |
| 4   | M     | 29  | ILE  |
| 4   | M     | 74  | LEU  |
| 4   | M     | 163 | PRO  |
| 4   | M     | 180 | HIS  |
| 4   | M     | 194 | PHE  |
| 4   | M     | 213 | LEU  |
| 4   | M     | 214 | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 297 | GLN  |
| 2   | H     | 58  | GLN  |
| 2   | H     | 102 | GLN  |
| 2   | H     | 220 | ASN  |
| 3   | L     | 183 | ASN  |
| 3   | L     | 213 | ASN  |
| 3   | L     | 239 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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   | FME  | H     | 1[A] | -    | 8,9,10       | 1.21 | 1 (12%)  | 8,9,11      | 2.94 | 2 (25%)  |
| 2   | FME  | H     | 1[B] | -    | 8,9,10       | 0.96 | 1 (12%)  | 8,9,11      | 2.95 | 2 (25%)  |

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   | FME  | H     | 1[A] | -    | -       | 3/7/9/11 | -     |
| 2   | FME  | H     | 1[B] | -    | -       | 4/7/9/11 | -     |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2   | H     | 1[A] | FME  | CN-N  | 2.29 | 1.40        | 1.33     |
| 2   | H     | 1[B] | FME  | CN-N  | 2.01 | 1.39        | 1.33     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | H     | 1[B] | FME  | CA-N-CN | -7.48 | 111.32      | 122.82   |
| 2   | H     | 1[A] | FME  | CA-N-CN | -7.16 | 111.81      | 122.82   |
| 2   | H     | 1[A] | FME  | CB-CA-N | 2.97  | 115.93      | 110.52   |
| 2   | H     | 1[B] | FME  | CB-CA-N | -2.60 | 105.78      | 110.52   |

There are no chirality outliers.

All (7) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 2   | H     | 1[A] | FME  | O1-CN-N-CA  |
| 2   | H     | 1[A] | FME  | CB-CA-N-CN  |
| 2   | H     | 1[B] | FME  | O1-CN-N-CA  |
| 2   | H     | 1[A] | FME  | CB-CG-SD-CE |
| 2   | H     | 1[B] | FME  | CB-CA-N-CN  |
| 2   | H     | 1[B] | FME  | CB-CG-SD-CE |
| 2   | H     | 1[B] | FME  | CA-CB-CG-SD |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 152 ligands modelled in this entry, 1 is monoatomic - leaving 151 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 8   | SO4  | C     | 348 | -    | 4,4,4        | 0.50 | 0           | 6,6,6       | 0.40 | 0           |
| 5   | HEC  | C     | 402 | 1    | 50,50,50     | 1.41 | 9 (18%)     | 68,82,82    | 1.34 | 9 (13%)     |
| 8   | SO4  | C     | 341 | -    | 4,4,4        | 0.45 | 0           | 6,6,6       | 0.27 | 0           |
| 8   | SO4  | C     | 353 | -    | 4,4,4        | 0.57 | 0           | 6,6,6       | 0.28 | 0           |
| 10  | GOL  | C     | 367 | -    | 5,5,5        | 0.25 | 0           | 5,5,5       | 1.16 | 0           |
| 8   | SO4  | M     | 324 | -    | 4,4,4        | 0.40 | 0           | 6,6,6       | 0.88 | 0           |
| 8   | SO4  | C     | 350 | -    | 4,4,4        | 0.47 | 0           | 6,6,6       | 0.14 | 0           |
| 10  | GOL  | L     | 282 | -    | 5,5,5        | 0.90 | 0           | 5,5,5       | 1.25 | 1 (20%)     |
| 17  | HTH  | M     | 332 | -    | 9,9,9        | 0.44 | 0           | 10,10,10    | 1.19 | 1 (10%)     |
| 8   | SO4  | C     | 339 | -    | 4,4,4        | 0.42 | 0           | 6,6,6       | 0.41 | 0           |
| 8   | SO4  | H     | 259 | -    | 4,4,4        | 0.36 | 0           | 6,6,6       | 0.43 | 0           |
| 6   | LDA  | L     | 712 | -    | 13,15,15     | 2.07 | 2 (15%)     | 14,17,17    | 0.35 | 0           |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | HTO  | H     | 273    | -    | 9,9,9        | 0.45 | 0        | 10,10,10    | 1.23 | 1 (10%)  |
| 8   | SO4  | C     | 351    | -    | 4,4,4        | 0.42 | 0        | 6,6,6       | 0.17 | 0        |
| 8   | SO4  | C     | 337[A] | -    | 4,4,4        | 0.47 | 0        | 6,6,6       | 0.21 | 0        |
| 10  | GOL  | H     | 279    | -    | 5,5,5        | 0.39 | 0        | 5,5,5       | 0.57 | 0        |
| 8   | SO4  | C     | 340    | -    | 4,4,4        | 0.45 | 0        | 6,6,6       | 0.67 | 0        |
| 10  | GOL  | C     | 368    | -    | 5,5,5        | 0.15 | 0        | 5,5,5       | 0.74 | 0        |
| 10  | GOL  | H     | 288    | -    | 5,5,5        | 0.39 | 0        | 5,5,5       | 0.38 | 0        |
| 6   | LDA  | L     | 710    | -    | 13,15,15     | 2.07 | 2 (15%)  | 14,17,17    | 0.48 | 0        |
| 12  | BPB  | M     | 402    | -    | 57,70,70     | 1.24 | 5 (8%)   | 55,101,101  | 1.71 | 10 (18%) |
| 10  | GOL  | H     | 276[A] | -    | 5,5,5        | 0.85 | 0        | 5,5,5       | 0.59 | 0        |
| 8   | SO4  | H     | 269    | -    | 4,4,4        | 0.47 | 0        | 6,6,6       | 0.20 | 0        |
| 8   | SO4  | M     | 330    | -    | 4,4,4        | 0.52 | 0        | 6,6,6       | 0.18 | 0        |
| 6   | LDA  | L     | 724    | -    | 13,15,15     | 2.28 | 2 (15%)  | 14,17,17    | 0.59 | 0        |
| 11  | BCB  | L     | 401    | 3    | 68,74,74     | 0.97 | 1 (1%)   | 77,115,115  | 2.14 | 17 (22%) |
| 8   | SO4  | M     | 328    | -    | 4,4,4        | 0.40 | 0        | 6,6,6       | 0.25 | 0        |
| 10  | GOL  | M     | 339    | -    | 5,5,5        | 0.26 | 0        | 5,5,5       | 0.35 | 0        |
| 10  | GOL  | H     | 290    | -    | 5,5,5        | 0.35 | 0        | 5,5,5       | 0.56 | 0        |
| 5   | HEC  | C     | 401    | 1    | 50,50,50     | 1.64 | 16 (32%) | 68,82,82    | 1.60 | 14 (20%) |
| 8   | SO4  | M     | 325    | -    | 4,4,4        | 0.25 | 0        | 6,6,6       | 0.60 | 0        |
| 11  | BCB  | M     | 400    | 4    | 68,74,74     | 1.17 | 6 (8%)   | 77,115,115  | 2.23 | 17 (22%) |
| 10  | GOL  | H     | 276[B] | -    | 5,5,5        | 0.84 | 0        | 5,5,5       | 0.98 | 0        |
| 10  | GOL  | M     | 335    | -    | 5,5,5        | 0.46 | 0        | 5,5,5       | 0.38 | 0        |
| 5   | HEC  | C     | 403    | 1    | 50,50,50     | 1.70 | 15 (30%) | 68,82,82    | 1.32 | 9 (13%)  |
| 8   | SO4  | H     | 266    | -    | 4,4,4        | 0.46 | 0        | 6,6,6       | 0.38 | 0        |
| 10  | GOL  | C     | 363    | -    | 5,5,5        | 0.82 | 0        | 5,5,5       | 1.12 | 0        |
| 9   | HTO  | L     | 276    | -    | 9,9,9        | 0.49 | 0        | 10,10,10    | 1.52 | 2 (20%)  |
| 10  | GOL  | H     | 286    | -    | 5,5,5        | 0.26 | 0        | 5,5,5       | 0.61 | 0        |
| 10  | GOL  | M     | 340    | -    | 5,5,5        | 0.47 | 0        | 5,5,5       | 0.61 | 0        |
| 8   | SO4  | H     | 262    | -    | 4,4,4        | 0.43 | 0        | 6,6,6       | 0.42 | 0        |
| 10  | GOL  | H     | 291    | -    | 5,5,5        | 0.38 | 0        | 5,5,5       | 0.45 | 0        |
| 12  | BPB  | L     | 402    | -    | 57,70,70     | 1.22 | 4 (7%)   | 55,101,101  | 2.36 | 14 (25%) |
| 10  | GOL  | H     | 280    | -    | 5,5,5        | 0.75 | 0        | 5,5,5       | 1.15 | 1 (20%)  |
| 10  | GOL  | C     | 364    | -    | 5,5,5        | 0.57 | 0        | 5,5,5       | 1.01 | 0        |
| 10  | GOL  | C     | 365    | -    | 5,5,5        | 0.36 | 0        | 5,5,5       | 0.38 | 0        |
| 9   | HTO  | C     | 358[A] | -    | 9,9,9        | 0.75 | 0        | 10,10,10    | 2.65 | 4 (40%)  |
| 6   | LDA  | H     | 719    | -    | 13,15,15     | 2.09 | 2 (15%)  | 14,17,17    | 0.53 | 0        |
| 6   | LDA  | M     | 705    | -    | 13,15,15     | 1.96 | 2 (15%)  | 14,17,17    | 0.53 | 0        |
| 10  | GOL  | C     | 360    | -    | 5,5,5        | 0.26 | 0        | 5,5,5       | 0.67 | 0        |
| 8   | SO4  | H     | 263    | -    | 4,4,4        | 0.47 | 0        | 6,6,6       | 0.28 | 0        |
| 8   | SO4  | C     | 345    | -    | 4,4,4        | 0.43 | 0        | 6,6,6       | 0.29 | 0        |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 8   | SO4  | C     | 338    | -    | 4,4,4        | 0.51 | 0        | 6,6,6       | 0.44 | 0        |
| 10  | GOL  | C     | 371    | -    | 5,5,5        | 0.35 | 0        | 5,5,5       | 0.83 | 0        |
| 10  | GOL  | L     | 286    | -    | 5,5,5        | 0.21 | 0        | 5,5,5       | 0.84 | 0        |
| 8   | SO4  | M     | 331    | -    | 4,4,4        | 0.45 | 0        | 6,6,6       | 0.17 | 0        |
| 10  | GOL  | H     | 275    | -    | 5,5,5        | 0.68 | 0        | 5,5,5       | 0.40 | 0        |
| 10  | GOL  | C     | 375    | -    | 5,5,5        | 0.29 | 0        | 5,5,5       | 0.21 | 0        |
| 6   | LDA  | H     | 701    | -    | 13,15,15     | 1.55 | 2 (15%)  | 14,17,17    | 0.93 | 0        |
| 9   | HTO  | C     | 357    | -    | 9,9,9        | 0.61 | 0        | 10,10,10    | 0.77 | 0        |
| 10  | GOL  | L     | 288    | -    | 5,5,5        | 0.15 | 0        | 5,5,5       | 0.67 | 0        |
| 13  | UQ9  | L     | 503    | -    | 23,23,58     | 2.20 | 9 (39%)  | 30,31,73    | 1.52 | 5 (16%)  |
| 10  | GOL  | C     | 374[B] | -    | 5,5,5        | 0.35 | 0        | 5,5,5       | 0.42 | 0        |
| 8   | SO4  | H     | 267    | -    | 4,4,4        | 0.37 | 0        | 6,6,6       | 0.20 | 0        |
| 6   | LDA  | L     | 723    | -    | 13,15,15     | 2.38 | 2 (15%)  | 14,17,17    | 0.78 | 0        |
| 10  | GOL  | C     | 372    | -    | 5,5,5        | 0.29 | 0        | 5,5,5       | 0.67 | 0        |
| 8   | SO4  | C     | 354    | -    | 4,4,4        | 0.37 | 0        | 6,6,6       | 0.38 | 0        |
| 7   | DGA  | C     | 730    | 1    | 36,36,43     | 0.87 | 2 (5%)   | 38,38,45    | 1.43 | 6 (15%)  |
| 9   | HTO  | C     | 356    | -    | 9,9,9        | 0.79 | 0        | 10,10,10    | 1.78 | 2 (20%)  |
| 6   | LDA  | C     | 722    | -    | 13,15,15     | 2.19 | 2 (15%)  | 14,17,17    | 0.58 | 0        |
| 10  | GOL  | H     | 287    | -    | 5,5,5        | 0.32 | 0        | 5,5,5       | 0.12 | 0        |
| 10  | GOL  | C     | 377    | -    | 5,5,5        | 0.18 | 0        | 5,5,5       | 0.37 | 0        |
| 10  | GOL  | M     | 338    | -    | 5,5,5        | 0.42 | 0        | 5,5,5       | 0.51 | 0        |
| 10  | GOL  | C     | 370    | -    | 5,5,5        | 0.27 | 0        | 5,5,5       | 0.25 | 0        |
| 10  | GOL  | M     | 334    | -    | 5,5,5        | 0.15 | 0        | 5,5,5       | 0.32 | 0        |
| 8   | SO4  | C     | 349    | -    | 4,4,4        | 0.55 | 0        | 6,6,6       | 0.20 | 0        |
| 10  | GOL  | H     | 289    | -    | 5,5,5        | 0.34 | 0        | 5,5,5       | 0.27 | 0        |
| 8   | SO4  | C     | 346    | -    | 4,4,4        | 0.49 | 0        | 6,6,6       | 0.40 | 0        |
| 10  | GOL  | H     | 281    | -    | 5,5,5        | 0.57 | 0        | 5,5,5       | 0.38 | 0        |
| 10  | GOL  | H     | 284    | -    | 5,5,5        | 0.37 | 0        | 5,5,5       | 0.87 | 0        |
| 10  | GOL  | C     | 373    | -    | 5,5,5        | 0.36 | 0        | 5,5,5       | 0.29 | 0        |
| 8   | SO4  | H     | 261[A] | -    | 4,4,4        | 0.50 | 0        | 6,6,6       | 0.34 | 0        |
| 8   | SO4  | C     | 344    | -    | 4,4,4        | 0.51 | 0        | 6,6,6       | 0.19 | 0        |
| 9   | HTO  | H     | 272    | -    | 9,9,9        | 0.75 | 0        | 10,10,10    | 1.74 | 4 (40%)  |
| 8   | SO4  | H     | 265    | -    | 4,4,4        | 0.52 | 0        | 6,6,6       | 0.32 | 0        |
| 6   | LDA  | L     | 708    | -    | 13,15,15     | 1.82 | 1 (7%)   | 14,17,17    | 1.25 | 2 (14%)  |
| 6   | LDA  | M     | 704    | -    | 13,15,15     | 2.45 | 2 (15%)  | 14,17,17    | 1.53 | 3 (21%)  |
| 8   | SO4  | C     | 342    | -    | 4,4,4        | 0.48 | 0        | 6,6,6       | 0.22 | 0        |
| 8   | SO4  | M     | 327    | -    | 4,4,4        | 0.51 | 0        | 6,6,6       | 0.21 | 0        |
| 6   | LDA  | M     | 713    | -    | 13,15,15     | 2.00 | 2 (15%)  | 14,17,17    | 0.71 | 0        |
| 6   | LDA  | M     | 714    | -    | 13,15,15     | 2.38 | 2 (15%)  | 14,17,17    | 0.36 | 0        |
| 9   | HTO  | L     | 277    | -    | 9,9,9        | 0.46 | 0        | 10,10,10    | 1.32 | 1 (10%)  |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | LDA  | M     | 717    | -    | 13,15,15     | 2.01 | 2 (15%)  | 14,17,17    | 0.59 | 0        |
| 6   | LDA  | L     | 702    | -    | 13,15,15     | 2.15 | 2 (15%)  | 14,17,17    | 0.63 | 0        |
| 6   | LDA  | M     | 715    | -    | 13,15,15     | 1.96 | 1 (7%)   | 14,17,17    | 0.44 | 0        |
| 8   | SO4  | H     | 271    | -    | 4,4,4        | 0.45 | 0        | 6,6,6       | 0.11 | 0        |
| 10  | GOL  | C     | 359    | -    | 5,5,5        | 0.85 | 0        | 5,5,5       | 0.89 | 0        |
| 10  | GOL  | C     | 366    | -    | 5,5,5        | 0.48 | 0        | 5,5,5       | 0.44 | 0        |
| 10  | GOL  | L     | 283    | -    | 5,5,5        | 0.44 | 0        | 5,5,5       | 0.58 | 0        |
| 8   | SO4  | H     | 264    | -    | 4,4,4        | 0.43 | 0        | 6,6,6       | 0.16 | 0        |
| 8   | SO4  | L     | 274    | -    | 4,4,4        | 0.40 | 0        | 6,6,6       | 0.34 | 0        |
| 10  | GOL  | C     | 369    | -    | 5,5,5        | 0.40 | 0        | 5,5,5       | 0.66 | 0        |
| 9   | HTO  | L     | 280    | -    | 9,9,9        | 0.44 | 0        | 10,10,10    | 1.00 | 1 (10%)  |
| 10  | GOL  | L     | 287    | -    | 5,5,5        | 0.36 | 0        | 5,5,5       | 0.64 | 0        |
| 8   | SO4  | H     | 261[B] | -    | 4,4,4        | 0.36 | 0        | 6,6,6       | 0.43 | 0        |
| 10  | GOL  | M     | 337    | -    | 5,5,5        | 0.34 | 0        | 5,5,5       | 0.38 | 0        |
| 9   | HTO  | M     | 333    | -    | 9,9,9        | 0.51 | 0        | 10,10,10    | 2.66 | 4 (40%)  |
| 11  | BCB  | L     | 400    | 3    | 68,74,74     | 0.96 | 5 (7%)   | 77,115,115  | 2.16 | 17 (22%) |
| 10  | GOL  | C     | 378    | -    | 5,5,5        | 0.34 | 0        | 5,5,5       | 0.18 | 0        |
| 10  | GOL  | H     | 277    | -    | 5,5,5        | 0.42 | 0        | 5,5,5       | 0.58 | 0        |
| 10  | GOL  | C     | 361    | -    | 5,5,5        | 0.60 | 0        | 5,5,5       | 1.15 | 1 (20%)  |
| 15  | MQ9  | M     | 501    | -    | 59,59,59     | 2.31 | 25 (42%) | 73,75,75    | 1.20 | 8 (10%)  |
| 16  | NS5  | M     | 600    | -    | 39,39,39     | 1.60 | 11 (28%) | 46,46,46    | 2.79 | 15 (32%) |
| 10  | GOL  | L     | 281    | -    | 5,5,5        | 0.19 | 0        | 5,5,5       | 0.48 | 0        |
| 8   | SO4  | M     | 326    | -    | 4,4,4        | 0.29 | 0        | 6,6,6       | 0.45 | 0        |
| 10  | GOL  | H     | 278    | -    | 5,5,5        | 0.49 | 0        | 5,5,5       | 0.83 | 0        |
| 6   | LDA  | L     | 709    | -    | 13,15,15     | 1.93 | 2 (15%)  | 14,17,17    | 0.46 | 0        |
| 13  | UQ9  | L     | 502    | -    | 58,58,58     | 2.28 | 24 (41%) | 72,73,73    | 1.55 | 14 (19%) |
| 8   | SO4  | H     | 260    | -    | 4,4,4        | 0.43 | 0        | 6,6,6       | 0.22 | 0        |
| 8   | SO4  | M     | 329    | -    | 4,4,4        | 0.40 | 0        | 6,6,6       | 0.33 | 0        |
| 6   | LDA  | M     | 706    | -    | 13,15,15     | 2.00 | 2 (15%)  | 14,17,17    | 0.57 | 0        |
| 11  | BCB  | M     | 401    | 4    | 68,74,74     | 1.17 | 7 (10%)  | 77,115,115  | 2.39 | 21 (27%) |
| 10  | GOL  | H     | 285    | -    | 5,5,5        | 0.18 | 0        | 5,5,5       | 0.62 | 0        |
| 10  | GOL  | L     | 285    | -    | 5,5,5        | 0.57 | 0        | 5,5,5       | 0.78 | 0        |
| 10  | GOL  | M     | 341    | -    | 5,5,5        | 0.39 | 0        | 5,5,5       | 0.25 | 0        |
| 8   | SO4  | C     | 347    | -    | 4,4,4        | 0.64 | 0        | 6,6,6       | 0.21 | 0        |
| 10  | GOL  | H     | 283    | 2    | 5,5,5        | 0.19 | 0        | 5,5,5       | 1.05 | 0        |
| 10  | GOL  | L     | 284    | -    | 5,5,5        | 0.38 | 0        | 5,5,5       | 0.53 | 0        |
| 6   | LDA  | H     | 718[B] | -    | 13,15,15     | 2.06 | 2 (15%)  | 14,17,17    | 0.61 | 0        |
| 6   | LDA  | H     | 720    | -    | 13,15,15     | 2.38 | 2 (15%)  | 14,17,17    | 0.76 | 0        |
| 6   | LDA  | C     | 716    | -    | 13,15,15     | 1.91 | 1 (7%)   | 14,17,17    | 0.67 | 0        |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | LDA  | L     | 703    | -    | 13,15,15     | 2.40 | 2 (15%)  | 14,17,17    | 0.57 | 0        |
| 8   | SO4  | C     | 343    | -    | 4,4,4        | 0.24 | 0        | 6,6,6       | 0.80 | 0        |
| 10  | GOL  | C     | 362    | -    | 5,5,5        | 0.72 | 0        | 5,5,5       | 0.89 | 0        |
| 10  | GOL  | H     | 282    | -    | 5,5,5        | 0.39 | 0        | 5,5,5       | 0.22 | 0        |
| 6   | LDA  | M     | 707    | -    | 13,15,15     | 2.11 | 2 (15%)  | 14,17,17    | 0.89 | 0        |
| 8   | SO4  | H     | 268    | -    | 4,4,4        | 0.40 | 0        | 6,6,6       | 0.15 | 0        |
| 9   | HTO  | L     | 279    | -    | 9,9,9        | 0.42 | 0        | 10,10,10    | 1.45 | 1 (10%)  |
| 6   | LDA  | L     | 711    | -    | 13,15,15     | 2.06 | 2 (15%)  | 14,17,17    | 0.60 | 0        |
| 9   | HTO  | L     | 278    | -    | 9,9,9        | 0.68 | 0        | 10,10,10    | 1.64 | 3 (30%)  |
| 9   | HTO  | H     | 274[A] | -    | 9,9,9        | 0.33 | 0        | 10,10,10    | 0.78 | 0        |
| 6   | LDA  | H     | 721    | -    | 13,15,15     | 1.97 | 2 (15%)  | 14,17,17    | 0.59 | 0        |
| 8   | SO4  | C     | 337[B] | -    | 4,4,4        | 0.45 | 0        | 6,6,6       | 0.21 | 0        |
| 8   | SO4  | C     | 352    | -    | 4,4,4        | 0.41 | 0        | 6,6,6       | 0.17 | 0        |
| 8   | SO4  | H     | 270    | -    | 4,4,4        | 0.44 | 0        | 6,6,6       | 0.18 | 0        |
| 10  | GOL  | C     | 376    | -    | 5,5,5        | 0.34 | 0        | 5,5,5       | 0.32 | 0        |
| 10  | GOL  | M     | 342    | -    | 5,5,5        | 0.41 | 0        | 5,5,5       | 0.71 | 0        |
| 8   | SO4  | L     | 275    | -    | 4,4,4        | 0.42 | 0        | 6,6,6       | 0.15 | 0        |
| 5   | HEC  | C     | 404    | 1    | 50,50,50     | 1.34 | 6 (12%)  | 68,82,82    | 1.59 | 17 (25%) |
| 9   | HTO  | C     | 355    | -    | 9,9,9        | 0.58 | 0        | 10,10,10    | 1.65 | 3 (30%)  |
| 10  | GOL  | M     | 336    | -    | 5,5,5        | 0.18 | 0        | 5,5,5       | 1.09 | 0        |

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   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 5   | HEC  | C     | 402 | 1    | 1/1/3/7 | 9/14/54/54   | -       |
| 10  | GOL  | C     | 367 | -    | -       | 3/4/4/4      | -       |
| 17  | HTH  | M     | 332 | -    | -       | 7/10/10/10   | -       |
| 10  | GOL  | L     | 282 | -    | -       | 2/4/4/4      | -       |
| 6   | LDA  | L     | 712 | -    | -       | 7/13/13/13   | -       |
| 9   | HTO  | H     | 273 | -    | -       | 4/10/10/10   | -       |
| 10  | GOL  | H     | 279 | -    | -       | 0/4/4/4      | -       |
| 10  | GOL  | C     | 368 | -    | -       | 4/4/4/4      | -       |
| 10  | GOL  | H     | 288 | -    | -       | 2/4/4/4      | -       |
| 6   | LDA  | L     | 710 | -    | -       | 8/13/13/13   | -       |
| 12  | BPB  | M     | 402 | -    | -       | 8/37/105/105 | 0/5/6/6 |

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| Mol | Type | Chain | Res    | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 10  | GOL  | H     | 276[A] | -    | -         | 4/4/4/4       | -       |
| 11  | BCB  | L     | 401    | 3    | 3/3/21/26 | 6/41/137/137  | -       |
| 6   | LDA  | L     | 724    | -    | -         | 6/13/13/13    | -       |
| 10  | GOL  | M     | 339    | -    | -         | 2/4/4/4       | -       |
| 10  | GOL  | H     | 290    | -    | -         | 2/4/4/4       | -       |
| 5   | HEC  | C     | 401    | 1    | 1/1/3/7   | 7/14/54/54    | -       |
| 11  | BCB  | M     | 400    | 4    | 3/3/21/26 | 11/41/137/137 | -       |
| 10  | GOL  | H     | 276[B] | -    | -         | 2/4/4/4       | -       |
| 10  | GOL  | M     | 335    | -    | -         | 0/4/4/4       | -       |
| 5   | HEC  | C     | 403    | 1    | 1/1/3/7   | 4/14/54/54    | -       |
| 10  | GOL  | C     | 363    | -    | -         | 0/4/4/4       | -       |
| 9   | HTO  | L     | 276    | -    | -         | 6/10/10/10    | -       |
| 10  | GOL  | H     | 286    | -    | -         | 3/4/4/4       | -       |
| 10  | GOL  | M     | 340    | -    | -         | 2/4/4/4       | -       |
| 10  | GOL  | H     | 291    | -    | -         | 2/4/4/4       | -       |
| 12  | BPB  | L     | 402    | -    | -         | 3/37/105/105  | 0/5/6/6 |
| 10  | GOL  | H     | 280    | -    | -         | 2/4/4/4       | -       |
| 10  | GOL  | C     | 364    | -    | -         | 3/4/4/4       | -       |
| 10  | GOL  | C     | 365    | -    | -         | 2/4/4/4       | -       |
| 9   | HTO  | C     | 358[A] | -    | -         | 10/10/10/10   | -       |
| 6   | LDA  | H     | 719    | -    | -         | 8/13/13/13    | -       |
| 6   | LDA  | M     | 705    | -    | -         | 6/13/13/13    | -       |
| 10  | GOL  | C     | 360    | -    | -         | 0/4/4/4       | -       |
| 10  | GOL  | C     | 371    | -    | -         | 0/4/4/4       | -       |
| 10  | GOL  | L     | 286    | -    | -         | 4/4/4/4       | -       |
| 10  | GOL  | H     | 275    | -    | -         | 2/4/4/4       | -       |
| 10  | GOL  | C     | 375    | -    | -         | 0/4/4/4       | -       |
| 6   | LDA  | H     | 701    | -    | -         | 4/13/13/13    | -       |
| 9   | HTO  | C     | 357    | -    | -         | 6/10/10/10    | -       |
| 10  | GOL  | L     | 288    | -    | -         | 2/4/4/4       | -       |
| 13  | UQ9  | L     | 503    | -    | -         | 3/15/39/81    | 0/1/1/1 |
| 10  | GOL  | C     | 374[B] | -    | -         | 4/4/4/4       | -       |
| 6   | LDA  | L     | 723    | -    | -         | 8/13/13/13    | -       |
| 10  | GOL  | C     | 372    | -    | -         | 2/4/4/4       | -       |
| 7   | DGA  | C     | 730    | 1    | -         | 27/37/37/45   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 9   | HTO  | C     | 356 | -    | -         | 8/10/10/10   | -       |
| 6   | LDA  | C     | 722 | -    | -         | 9/13/13/13   | -       |
| 10  | GOL  | H     | 287 | -    | -         | 4/4/4/4      | -       |
| 10  | GOL  | C     | 377 | -    | -         | 2/4/4/4      | -       |
| 10  | GOL  | M     | 338 | -    | -         | 4/4/4/4      | -       |
| 10  | GOL  | C     | 370 | -    | -         | 2/4/4/4      | -       |
| 10  | GOL  | M     | 334 | -    | -         | 4/4/4/4      | -       |
| 10  | GOL  | H     | 289 | -    | -         | 4/4/4/4      | -       |
| 10  | GOL  | H     | 281 | -    | -         | 3/4/4/4      | -       |
| 10  | GOL  | H     | 284 | -    | -         | 2/4/4/4      | -       |
| 10  | GOL  | C     | 373 | -    | -         | 2/4/4/4      | -       |
| 9   | HTO  | H     | 272 | -    | -         | 1/10/10/10   | -       |
| 6   | LDA  | L     | 708 | -    | -         | 8/13/13/13   | -       |
| 6   | LDA  | M     | 704 | -    | -         | 5/13/13/13   | -       |
| 6   | LDA  | M     | 713 | -    | -         | 4/13/13/13   | -       |
| 6   | LDA  | M     | 714 | -    | -         | 8/13/13/13   | -       |
| 9   | HTO  | L     | 277 | -    | -         | 0/10/10/10   | -       |
| 6   | LDA  | M     | 717 | -    | -         | 2/13/13/13   | -       |
| 6   | LDA  | L     | 702 | -    | -         | 7/13/13/13   | -       |
| 6   | LDA  | M     | 715 | -    | -         | 5/13/13/13   | -       |
| 10  | GOL  | C     | 359 | -    | -         | 1/4/4/4      | -       |
| 10  | GOL  | C     | 366 | -    | -         | 2/4/4/4      | -       |
| 10  | GOL  | L     | 283 | -    | -         | 2/4/4/4      | -       |
| 10  | GOL  | C     | 369 | -    | -         | 2/4/4/4      | -       |
| 9   | HTO  | L     | 280 | -    | -         | 5/10/10/10   | -       |
| 10  | GOL  | L     | 287 | -    | -         | 0/4/4/4      | -       |
| 10  | GOL  | M     | 337 | -    | -         | 2/4/4/4      | -       |
| 9   | HTO  | M     | 333 | -    | -         | 7/10/10/10   | -       |
| 11  | BCB  | L     | 400 | 3    | 3/3/21/26 | 7/41/137/137 | -       |
| 10  | GOL  | C     | 378 | -    | -         | 2/4/4/4      | -       |
| 10  | GOL  | H     | 277 | -    | -         | 2/4/4/4      | -       |
| 10  | GOL  | C     | 361 | -    | -         | 0/4/4/4      | -       |
| 15  | MQ9  | M     | 501 | -    | -         | 2/53/73/73   | 0/2/2/2 |
| 16  | NS5  | M     | 600 | -    | -         | 8/43/43/43   | -       |
| 10  | GOL  | L     | 281 | -    | -         | 0/4/4/4      | -       |

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| Mol | Type | Chain | Res    | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|--------|------|-----------|---------------|---------|
| 10  | GOL  | H     | 278    | -    | -         | 2/4/4/4       | -       |
| 6   | LDA  | L     | 709    | -    | -         | 6/13/13/13    | -       |
| 13  | UQ9  | L     | 502    | -    | -         | 17/57/81/81   | 0/1/1/1 |
| 6   | LDA  | M     | 706    | -    | -         | 8/13/13/13    | -       |
| 11  | BCB  | M     | 401    | 4    | 3/3/21/26 | 10/41/137/137 | -       |
| 10  | GOL  | H     | 285    | -    | -         | 3/4/4/4       | -       |
| 10  | GOL  | L     | 285    | -    | -         | 2/4/4/4       | -       |
| 10  | GOL  | M     | 341    | -    | -         | 0/4/4/4       | -       |
| 10  | GOL  | H     | 283    | 2    | -         | 4/4/4/4       | -       |
| 10  | GOL  | L     | 284    | -    | -         | 4/4/4/4       | -       |
| 6   | LDA  | H     | 718[B] | -    | -         | 8/13/13/13    | -       |
| 6   | LDA  | H     | 720    | -    | -         | 6/13/13/13    | -       |
| 6   | LDA  | C     | 716    | -    | -         | 10/13/13/13   | -       |
| 6   | LDA  | L     | 703    | -    | -         | 6/13/13/13    | -       |
| 10  | GOL  | C     | 362    | -    | -         | 2/4/4/4       | -       |
| 10  | GOL  | H     | 282    | -    | -         | 2/4/4/4       | -       |
| 6   | LDA  | M     | 707    | -    | -         | 7/13/13/13    | -       |
| 9   | HTO  | L     | 279    | -    | -         | 3/10/10/10    | -       |
| 6   | LDA  | L     | 711    | -    | -         | 4/13/13/13    | -       |
| 9   | HTO  | L     | 278    | -    | -         | 4/10/10/10    | -       |
| 9   | HTO  | H     | 274[A] | -    | -         | 4/10/10/10    | -       |
| 6   | LDA  | H     | 721    | -    | -         | 10/13/13/13   | -       |
| 10  | GOL  | C     | 376    | -    | -         | 2/4/4/4       | -       |
| 10  | GOL  | M     | 342    | -    | -         | 4/4/4/4       | -       |
| 5   | HEC  | C     | 404    | 1    | 1/1/3/7   | 5/14/54/54    | -       |
| 9   | HTO  | C     | 355    | -    | -         | 4/10/10/10    | -       |
| 10  | GOL  | M     | 336    | -    | -         | 4/4/4/4       | -       |

All (190) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6   | M     | 704 | LDA  | O1-N1 | -7.60 | 1.23        | 1.42     |
| 6   | H     | 720 | LDA  | O1-N1 | -7.31 | 1.24        | 1.42     |
| 6   | M     | 714 | LDA  | O1-N1 | -7.26 | 1.24        | 1.42     |
| 6   | L     | 724 | LDA  | O1-N1 | -7.18 | 1.24        | 1.42     |
| 6   | M     | 707 | LDA  | O1-N1 | -7.03 | 1.24        | 1.42     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 6   | L     | 703    | LDA  | O1-N1   | -6.94 | 1.25        | 1.42     |
| 6   | L     | 710    | LDA  | O1-N1   | -6.85 | 1.25        | 1.42     |
| 6   | L     | 712    | LDA  | O1-N1   | -6.85 | 1.25        | 1.42     |
| 6   | L     | 702    | LDA  | O1-N1   | -6.78 | 1.25        | 1.42     |
| 6   | L     | 711    | LDA  | O1-N1   | -6.77 | 1.25        | 1.42     |
| 6   | L     | 723    | LDA  | O1-N1   | -6.65 | 1.25        | 1.42     |
| 6   | M     | 715    | LDA  | O1-N1   | -6.65 | 1.25        | 1.42     |
| 6   | H     | 718[B] | LDA  | O1-N1   | -6.53 | 1.26        | 1.42     |
| 6   | H     | 719    | LDA  | O1-N1   | -6.52 | 1.26        | 1.42     |
| 6   | M     | 713    | LDA  | O1-N1   | -6.51 | 1.26        | 1.42     |
| 6   | C     | 716    | LDA  | O1-N1   | -6.50 | 1.26        | 1.42     |
| 6   | L     | 708    | LDA  | O1-N1   | -6.46 | 1.26        | 1.42     |
| 6   | C     | 722    | LDA  | O1-N1   | -6.45 | 1.26        | 1.42     |
| 6   | L     | 709    | LDA  | O1-N1   | -6.41 | 1.26        | 1.42     |
| 6   | M     | 717    | LDA  | O1-N1   | -6.38 | 1.26        | 1.42     |
| 6   | M     | 706    | LDA  | O1-N1   | -6.33 | 1.26        | 1.42     |
| 6   | H     | 721    | LDA  | O1-N1   | -6.10 | 1.27        | 1.42     |
| 13  | L     | 502    | UQ9  | C7-C8   | -6.09 | 1.41        | 1.50     |
| 13  | L     | 503    | UQ9  | C7-C8   | -6.07 | 1.41        | 1.50     |
| 6   | M     | 705    | LDA  | O1-N1   | -6.07 | 1.27        | 1.42     |
| 6   | L     | 723    | LDA  | C1-N1   | -5.37 | 1.45        | 1.51     |
| 6   | L     | 703    | LDA  | C1-N1   | -5.06 | 1.46        | 1.51     |
| 6   | H     | 701    | LDA  | O1-N1   | -4.94 | 1.30        | 1.42     |
| 12  | M     | 402    | BPB  | C1B-C2B | 4.89  | 1.44        | 1.39     |
| 12  | L     | 402    | BPB  | C1B-C2B | 4.76  | 1.44        | 1.39     |
| 15  | M     | 501    | MQ9  | C7-C8   | -4.62 | 1.43        | 1.50     |
| 15  | M     | 501    | MQ9  | C6-C5   | 4.57  | 1.43        | 1.35     |
| 15  | M     | 501    | MQ9  | C2-C1   | -4.54 | 1.39        | 1.48     |
| 6   | M     | 714    | LDA  | C1-N1   | -4.50 | 1.46        | 1.51     |
| 6   | C     | 722    | LDA  | C1-N1   | -4.46 | 1.46        | 1.51     |
| 6   | H     | 720    | LDA  | C1-N1   | -4.38 | 1.47        | 1.51     |
| 6   | M     | 704    | LDA  | C1-N1   | -4.08 | 1.47        | 1.51     |
| 6   | L     | 724    | LDA  | C1-N1   | -3.87 | 1.47        | 1.51     |
| 15  | M     | 501    | MQ9  | C43-C44 | 3.84  | 1.41        | 1.33     |
| 15  | M     | 501    | MQ9  | C33-C34 | 3.78  | 1.41        | 1.33     |
| 13  | L     | 502    | UQ9  | C42-C43 | -3.69 | 1.39        | 1.50     |
| 6   | L     | 702    | LDA  | C1-N1   | -3.69 | 1.47        | 1.51     |
| 6   | H     | 719    | LDA  | C1-N1   | -3.65 | 1.47        | 1.51     |
| 11  | M     | 400    | BCB  | C4B-NB  | 3.62  | 1.42        | 1.37     |
| 13  | L     | 502    | UQ9  | C32-C33 | -3.57 | 1.39        | 1.50     |
| 6   | H     | 721    | LDA  | C1-N1   | -3.57 | 1.47        | 1.51     |
| 15  | M     | 501    | MQ9  | C8-C9   | 3.57  | 1.41        | 1.33     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 15  | M     | 501    | MQ9  | C5M-C5  | 3.55  | 1.58        | 1.50     |
| 5   | C     | 403    | HEC  | C4B-C3B | -3.55 | 1.39        | 1.45     |
| 13  | L     | 502    | UQ9  | C47-C48 | -3.53 | 1.39        | 1.50     |
| 15  | M     | 501    | MQ9  | C37-C38 | -3.50 | 1.39        | 1.50     |
| 13  | L     | 502    | UQ9  | C22-C23 | -3.48 | 1.39        | 1.50     |
| 15  | M     | 501    | MQ9  | C38-C39 | 3.48  | 1.41        | 1.33     |
| 6   | H     | 718[B] | LDA  | C1-N1   | -3.47 | 1.47        | 1.51     |
| 13  | L     | 502    | UQ9  | C8-C9   | 3.43  | 1.41        | 1.33     |
| 5   | C     | 401    | HEC  | FE-NB   | 3.43  | 2.05        | 1.94     |
| 5   | C     | 403    | HEC  | C2A-C3A | 3.43  | 1.44        | 1.36     |
| 6   | M     | 705    | LDA  | C1-N1   | -3.43 | 1.48        | 1.51     |
| 13  | L     | 502    | UQ9  | C27-C28 | -3.42 | 1.40        | 1.50     |
| 13  | L     | 502    | UQ9  | C12-C13 | -3.40 | 1.40        | 1.50     |
| 6   | M     | 717    | LDA  | C1-N1   | -3.38 | 1.48        | 1.51     |
| 15  | M     | 501    | MQ9  | C5-C4   | -3.37 | 1.39        | 1.47     |
| 15  | M     | 501    | MQ9  | C28-C29 | 3.35  | 1.40        | 1.33     |
| 6   | M     | 706    | LDA  | C1-N1   | -3.35 | 1.48        | 1.51     |
| 11  | M     | 401    | BCB  | O2D-CGD | 3.33  | 1.41        | 1.33     |
| 12  | M     | 402    | BPB  | C3A-C2A | 3.30  | 1.57        | 1.54     |
| 15  | M     | 501    | MQ9  | C27-C28 | -3.28 | 1.40        | 1.50     |
| 15  | M     | 501    | MQ9  | C47-C48 | -3.27 | 1.40        | 1.50     |
| 13  | L     | 503    | UQ9  | C8-C9   | 3.26  | 1.40        | 1.33     |
| 13  | L     | 502    | UQ9  | C4-C5   | -3.25 | 1.39        | 1.48     |
| 13  | L     | 503    | UQ9  | C12-C13 | -3.25 | 1.40        | 1.50     |
| 13  | L     | 502    | UQ9  | C28-C29 | 3.24  | 1.40        | 1.33     |
| 13  | L     | 502    | UQ9  | C38-C39 | 3.22  | 1.40        | 1.33     |
| 13  | L     | 502    | UQ9  | C6-C1   | 3.20  | 1.40        | 1.35     |
| 15  | M     | 501    | MQ9  | C32-C33 | -3.20 | 1.40        | 1.50     |
| 13  | L     | 502    | UQ9  | C18-C19 | 3.19  | 1.40        | 1.33     |
| 5   | C     | 403    | HEC  | C1D-ND  | -3.19 | 1.34        | 1.40     |
| 15  | M     | 501    | MQ9  | C22-C23 | -3.19 | 1.40        | 1.50     |
| 13  | L     | 502    | UQ9  | C3-C2   | -3.18 | 1.39        | 1.48     |
| 13  | L     | 502    | UQ9  | C17-C18 | -3.18 | 1.40        | 1.50     |
| 13  | L     | 502    | UQ9  | C37-C38 | -3.14 | 1.41        | 1.50     |
| 5   | C     | 401    | HEC  | C1A-C2A | -3.13 | 1.39        | 1.45     |
| 12  | M     | 402    | BPB  | C3D-C4D | -3.08 | 1.37        | 1.41     |
| 15  | M     | 501    | MQ9  | C18-C19 | 3.05  | 1.40        | 1.33     |
| 13  | L     | 503    | UQ9  | C6-C1   | 3.04  | 1.40        | 1.35     |
| 16  | M     | 600    | NS5  | C24-C25 | 3.03  | 1.52        | 1.43     |
| 15  | M     | 501    | MQ9  | C42-C43 | -3.01 | 1.41        | 1.50     |
| 6   | M     | 713    | LDA  | C1-N1   | -3.01 | 1.48        | 1.51     |
| 5   | C     | 401    | HEC  | C1D-ND  | -3.00 | 1.35        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | C     | 403 | HEC  | FE-ND   | 2.99  | 2.04        | 1.94     |
| 13  | L     | 502 | UQ9  | C13-C14 | 2.93  | 1.39        | 1.33     |
| 11  | M     | 400 | BCB  | CMD-C2D | 2.93  | 1.56        | 1.50     |
| 5   | C     | 401 | HEC  | C4B-C3B | -2.92 | 1.40        | 1.45     |
| 15  | M     | 501 | MQ9  | C12-C13 | -2.90 | 1.41        | 1.50     |
| 5   | C     | 401 | HEC  | FE-ND   | 2.89  | 2.03        | 1.94     |
| 16  | M     | 600 | NS5  | C23-C21 | 2.89  | 1.52        | 1.46     |
| 16  | M     | 600 | NS5  | C29-C30 | 2.88  | 1.52        | 1.43     |
| 5   | C     | 401 | HEC  | C4A-NA  | -2.88 | 1.34        | 1.39     |
| 11  | M     | 401 | BCB  | CAA-CBA | -2.88 | 1.44        | 1.52     |
| 13  | L     | 503 | UQ9  | C3-C2   | -2.84 | 1.40        | 1.48     |
| 15  | M     | 501 | MQ9  | C6-C1   | -2.84 | 1.40        | 1.47     |
| 13  | L     | 502 | UQ9  | C23-C24 | 2.83  | 1.39        | 1.33     |
| 6   | L     | 710 | LDA  | C1-N1   | -2.83 | 1.48        | 1.51     |
| 6   | L     | 711 | LDA  | C1-N1   | -2.82 | 1.48        | 1.51     |
| 13  | L     | 502 | UQ9  | C6-C5   | -2.81 | 1.38        | 1.46     |
| 11  | L     | 400 | BCB  | MG-ND   | -2.80 | 2.00        | 2.05     |
| 5   | C     | 402 | HEC  | C4A-C3A | -2.77 | 1.39        | 1.45     |
| 13  | L     | 502 | UQ9  | C48-C49 | 2.76  | 1.40        | 1.32     |
| 11  | L     | 401 | BCB  | CMA-C3A | 2.72  | 1.58        | 1.53     |
| 13  | L     | 502 | UQ9  | C33-C34 | 2.72  | 1.39        | 1.33     |
| 11  | L     | 400 | BCB  | O2D-CGD | 2.72  | 1.39        | 1.33     |
| 13  | L     | 503 | UQ9  | C4-C5   | -2.71 | 1.41        | 1.48     |
| 6   | M     | 707 | LDA  | C1-N1   | -2.69 | 1.48        | 1.51     |
| 5   | C     | 403 | HEC  | C4A-C3A | -2.69 | 1.40        | 1.45     |
| 6   | L     | 712 | LDA  | C1-N1   | -2.69 | 1.48        | 1.51     |
| 5   | C     | 403 | HEC  | FE-NA   | 2.68  | 2.04        | 1.95     |
| 11  | M     | 401 | BCB  | C1D-C2D | -2.65 | 1.40        | 1.45     |
| 7   | C     | 730 | DGA  | CG1-CG2 | 2.65  | 1.56        | 1.50     |
| 11  | M     | 401 | BCB  | C1B-NB  | 2.64  | 1.41        | 1.37     |
| 12  | L     | 402 | BPB  | C3D-CAD | -2.63 | 1.42        | 1.47     |
| 13  | L     | 502 | UQ9  | C43-C44 | 2.63  | 1.39        | 1.33     |
| 15  | M     | 501 | MQ9  | C17-C18 | -2.62 | 1.42        | 1.50     |
| 13  | L     | 503 | UQ9  | C13-C14 | 2.62  | 1.40        | 1.32     |
| 5   | C     | 404 | HEC  | C4D-C3D | -2.61 | 1.40        | 1.45     |
| 11  | M     | 401 | BCB  | MG-NB   | -2.61 | 2.00        | 2.05     |
| 15  | M     | 501 | MQ9  | C48-C49 | 2.59  | 1.40        | 1.32     |
| 5   | C     | 402 | HEC  | C1D-ND  | -2.57 | 1.35        | 1.40     |
| 5   | C     | 403 | HEC  | C1A-C2A | -2.56 | 1.40        | 1.45     |
| 12  | M     | 402 | BPB  | C3B-C4B | 2.55  | 1.45        | 1.41     |
| 16  | M     | 600 | NS5  | C28-C26 | 2.54  | 1.51        | 1.46     |
| 11  | M     | 400 | BCB  | C1B-NB  | 2.53  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | C     | 402 | HEC  | C1B-C2B | -2.52 | 1.39        | 1.44     |
| 12  | L     | 402 | BPB  | C1D-C2D | 2.50  | 1.42        | 1.39     |
| 5   | C     | 403 | HEC  | FE-NB   | 2.50  | 2.02        | 1.94     |
| 15  | M     | 501 | MQ9  | C41-C39 | 2.49  | 1.56        | 1.51     |
| 5   | C     | 402 | HEC  | C4A-NA  | -2.49 | 1.34        | 1.39     |
| 5   | C     | 402 | HEC  | C1D-C2D | -2.49 | 1.39        | 1.44     |
| 11  | M     | 400 | BCB  | CHB-C4A | 2.47  | 1.43        | 1.37     |
| 16  | M     | 600 | NS5  | C22-C21 | 2.47  | 1.55        | 1.50     |
| 15  | M     | 501 | MQ9  | C23-C24 | 2.46  | 1.38        | 1.33     |
| 16  | M     | 600 | NS5  | C16-C15 | 2.46  | 1.55        | 1.50     |
| 6   | L     | 709 | LDA  | C1-N1   | -2.45 | 1.49        | 1.51     |
| 5   | C     | 402 | HEC  | C4D-C3D | -2.45 | 1.40        | 1.45     |
| 11  | L     | 400 | BCB  | C1D-C2D | -2.44 | 1.40        | 1.45     |
| 5   | C     | 404 | HEC  | C4A-C3A | -2.44 | 1.40        | 1.45     |
| 5   | C     | 404 | HEC  | C1D-ND  | -2.44 | 1.36        | 1.40     |
| 5   | C     | 401 | HEC  | C4D-C3D | -2.43 | 1.40        | 1.45     |
| 16  | M     | 600 | NS5  | C19-C20 | 2.42  | 1.50        | 1.43     |
| 11  | M     | 400 | BCB  | C1D-C2D | -2.41 | 1.40        | 1.45     |
| 15  | M     | 501 | MQ9  | C46-C44 | 2.40  | 1.56        | 1.51     |
| 5   | C     | 403 | HEC  | FE-NC   | 2.40  | 2.03        | 1.95     |
| 5   | C     | 404 | HEC  | FE-NC   | 2.36  | 2.03        | 1.95     |
| 16  | M     | 600 | NS5  | C20-C21 | 2.35  | 1.41        | 1.35     |
| 5   | C     | 403 | HEC  | C4B-NB  | -2.34 | 1.36        | 1.40     |
| 16  | M     | 600 | NS5  | C13-C12 | 2.31  | 1.50        | 1.43     |
| 12  | L     | 402 | BPB  | C3B-C4B | 2.29  | 1.45        | 1.41     |
| 6   | H     | 701 | LDA  | C1-N1   | -2.26 | 1.49        | 1.51     |
| 13  | L     | 503 | UQ9  | C7-C6   | 2.24  | 1.55        | 1.51     |
| 15  | M     | 501 | MQ9  | O4-C4   | 2.23  | 1.27        | 1.23     |
| 5   | C     | 401 | HEC  | C1D-C2D | -2.23 | 1.40        | 1.44     |
| 11  | L     | 400 | BCB  | CMD-C2D | 2.22  | 1.55        | 1.50     |
| 11  | M     | 400 | BCB  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 5   | C     | 402 | HEC  | FE-NB   | 2.18  | 2.01        | 1.94     |
| 16  | M     | 600 | NS5  | C33-C31 | 2.17  | 1.55        | 1.51     |
| 5   | C     | 402 | HEC  | FE-ND   | 2.17  | 2.01        | 1.94     |
| 5   | C     | 401 | HEC  | O1D-CGD | 2.16  | 1.29        | 1.22     |
| 5   | C     | 401 | HEC  | C4B-NB  | -2.16 | 1.36        | 1.40     |
| 11  | L     | 400 | BCB  | MG-NC   | -2.16 | 2.01        | 2.06     |
| 5   | C     | 401 | HEC  | C2A-C3A | 2.14  | 1.41        | 1.36     |
| 13  | L     | 502 | UQ9  | C7-C6   | 2.14  | 1.55        | 1.51     |
| 5   | C     | 402 | HEC  | O2A-CGA | -2.13 | 1.23        | 1.30     |
| 5   | C     | 403 | HEC  | C1D-C2D | -2.13 | 1.40        | 1.44     |
| 16  | M     | 600 | NS5  | C34-C35 | 2.12  | 1.56        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | C     | 404 | HEC  | CHC-C1C | -2.12 | 1.34        | 1.39     |
| 5   | C     | 404 | HEC  | C4D-ND  | -2.10 | 1.34        | 1.38     |
| 13  | L     | 502 | UQ9  | C25-C24 | 2.10  | 1.55        | 1.50     |
| 5   | C     | 401 | HEC  | C4C-NC  | -2.07 | 1.35        | 1.39     |
| 5   | C     | 403 | HEC  | C1A-NA  | -2.07 | 1.35        | 1.39     |
| 12  | M     | 402 | BPB  | C3D-CAD | -2.06 | 1.43        | 1.47     |
| 5   | C     | 403 | HEC  | C1B-C2B | -2.06 | 1.40        | 1.44     |
| 5   | C     | 401 | HEC  | CMB-C2B | 2.05  | 1.55        | 1.50     |
| 13  | L     | 503 | UQ9  | C1-C2   | -2.04 | 1.40        | 1.47     |
| 7   | C     | 730 | DGA  | CA2-CA1 | 2.04  | 1.56        | 1.50     |
| 11  | M     | 401 | BCB  | MG-ND   | -2.04 | 2.01        | 2.05     |
| 5   | C     | 403 | HEC  | C3D-C2D | 2.04  | 1.41        | 1.36     |
| 5   | C     | 401 | HEC  | C3D-C2D | 2.03  | 1.41        | 1.36     |
| 5   | C     | 401 | HEC  | C4A-C3A | -2.03 | 1.41        | 1.45     |
| 11  | M     | 401 | BCB  | O2A-CGA | 2.01  | 1.39        | 1.33     |
| 5   | C     | 401 | HEC  | C1B-NB  | -2.01 | 1.34        | 1.38     |
| 5   | C     | 403 | HEC  | O2D-CGD | -2.01 | 1.24        | 1.30     |

All (228) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|--------|-------------|----------|
| 12  | L     | 402    | BPB  | C4D-CHA-CBD | -10.30 | 103.51      | 108.45   |
| 11  | L     | 401    | BCB  | C1D-ND-C4D  | 9.71   | 113.13      | 106.31   |
| 11  | M     | 400    | BCB  | C1D-ND-C4D  | 9.37   | 112.89      | 106.31   |
| 11  | L     | 400    | BCB  | C1D-ND-C4D  | 8.61   | 112.36      | 106.31   |
| 11  | M     | 401    | BCB  | C4A-NA-C1A  | 8.55   | 110.58      | 106.68   |
| 11  | L     | 401    | BCB  | C1C-NC-C4C  | -8.07  | 103.00      | 106.68   |
| 11  | M     | 400    | BCB  | C1C-NC-C4C  | -7.89  | 103.08      | 106.68   |
| 11  | M     | 401    | BCB  | O2D-CGD-CBD | 7.63   | 124.57      | 111.23   |
| 12  | L     | 402    | BPB  | C2B-C1B-NB  | -6.83  | 104.49      | 109.43   |
| 16  | M     | 600    | NS5  | C19-C20-C21 | -6.79  | 117.75      | 127.28   |
| 11  | M     | 401    | BCB  | O2D-CGD-O1D | -6.70  | 110.80      | 123.85   |
| 16  | M     | 600    | NS5  | C14-C15-C17 | -6.58  | 108.65      | 119.01   |
| 9   | M     | 333    | HTO  | C5-C4-C3    | -6.58  | 103.33      | 114.11   |
| 11  | L     | 400    | BCB  | C4A-NA-C1A  | 6.55   | 109.67      | 106.68   |
| 16  | M     | 600    | NS5  | C11-C10-C9  | 6.52   | 126.55      | 115.23   |
| 11  | M     | 401    | BCB  | C1D-ND-C4D  | 6.45   | 110.84      | 106.31   |
| 16  | M     | 600    | NS5  | C29-C30-C31 | -5.94  | 119.34      | 127.69   |
| 9   | C     | 358[A] | HTO  | C5-C4-C3    | -5.81  | 104.58      | 114.11   |
| 11  | M     | 401    | BCB  | C4D-C3D-CAD | -5.31  | 102.33      | 108.11   |
| 16  | M     | 600    | NS5  | C18-C19-C20 | 5.26   | 134.29      | 123.52   |
| 12  | L     | 402    | BPB  | C4A-C3A-C2A | -5.25  | 97.84       | 102.84   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 12  | M     | 402    | BPB  | C4D-CHA-CBD | -5.24 | 105.94      | 108.45   |
| 11  | M     | 400    | BCB  | C4A-NA-C1A  | 5.20  | 109.05      | 106.68   |
| 12  | M     | 402    | BPB  | C4A-C3A-C2A | -5.15 | 97.94       | 102.84   |
| 16  | M     | 600    | NS5  | C16-C15-C17 | 5.10  | 131.08      | 122.82   |
| 11  | L     | 400    | BCB  | C4D-C3D-CAD | -4.98 | 102.70      | 108.11   |
| 11  | M     | 400    | BCB  | C4D-C3D-CAD | -4.76 | 102.93      | 108.11   |
| 11  | L     | 401    | BCB  | C2D-C1D-ND  | -4.71 | 105.47      | 110.13   |
| 7   | C     | 730    | DGA  | CG2-OG2-CB1 | -4.60 | 111.15      | 117.78   |
| 16  | M     | 600    | NS5  | C24-C25-C26 | -4.58 | 120.85      | 127.28   |
| 11  | L     | 400    | BCB  | O2D-CGD-CBD | 4.35  | 118.84      | 111.23   |
| 13  | L     | 503    | UQ9  | C7-C8-C9    | 4.34  | 134.30      | 126.83   |
| 11  | L     | 400    | BCB  | CMD-C2D-C1D | 4.23  | 132.18      | 124.73   |
| 11  | M     | 401    | BCB  | CAA-C2A-C1A | -4.20 | 98.20       | 111.97   |
| 13  | L     | 502    | UQ9  | C25-C24-C26 | 4.18  | 122.49      | 115.23   |
| 9   | C     | 356    | HTO  | O3-C3-C2    | -4.18 | 100.80      | 109.57   |
| 6   | M     | 704    | LDA  | CM1-N1-C1   | -4.15 | 101.52      | 110.23   |
| 16  | M     | 600    | NS5  | C12-C13-C14 | -4.11 | 111.28      | 123.20   |
| 11  | L     | 400    | BCB  | C1C-NC-C4C  | -4.08 | 104.82      | 106.68   |
| 11  | M     | 400    | BCB  | CHA-C4D-ND  | 4.07  | 140.95      | 132.55   |
| 12  | L     | 402    | BPB  | C4B-NB-C1B  | 4.03  | 114.69      | 108.82   |
| 7   | C     | 730    | DGA  | OG2-CB1-CB2 | 4.00  | 120.13      | 111.48   |
| 11  | L     | 401    | BCB  | C3C-C4C-NC  | 3.99  | 115.38      | 110.45   |
| 12  | L     | 402    | BPB  | OBD-CAD-CBD | -3.98 | 119.98      | 125.82   |
| 12  | M     | 402    | BPB  | OBD-CAD-CBD | -3.95 | 120.03      | 125.82   |
| 11  | M     | 400    | BCB  | C1-C2-C3    | -3.94 | 119.73      | 126.20   |
| 16  | M     | 600    | NS5  | C6-C5-C4    | 3.94  | 122.07      | 115.23   |
| 12  | M     | 402    | BPB  | CMB-C2B-C3B | 3.85  | 132.37      | 124.68   |
| 13  | L     | 502    | UQ9  | C30-C29-C31 | 3.81  | 121.84      | 115.23   |
| 16  | M     | 600    | NS5  | C8-C7-C5    | -3.79 | 118.95      | 127.62   |
| 9   | C     | 358[A] | HTO  | O1-C1-C2    | -3.78 | 103.22      | 111.16   |
| 11  | M     | 400    | BCB  | C3C-C4C-NC  | 3.77  | 115.12      | 110.45   |
| 11  | L     | 401    | BCB  | CHA-C4D-ND  | 3.77  | 140.32      | 132.55   |
| 5   | C     | 401    | HEC  | C3C-C4C-NC  | 3.76  | 114.32      | 110.15   |
| 11  | M     | 401    | BCB  | C1-C2-C3    | -3.76 | 120.04      | 126.20   |
| 11  | L     | 401    | BCB  | C4D-C3D-CAD | -3.69 | 104.09      | 108.11   |
| 9   | L     | 277    | HTO  | C5-C4-C3    | -3.68 | 108.09      | 114.11   |
| 11  | L     | 400    | BCB  | O2A-CGA-O1A | -3.68 | 114.43      | 123.63   |
| 9   | C     | 358[A] | HTO  | O3-C3-C4    | -3.61 | 100.95      | 109.14   |
| 12  | L     | 402    | BPB  | O1D-CGD-CBD | -3.59 | 119.27      | 124.72   |
| 11  | L     | 401    | BCB  | C4-C3-C5    | 3.56  | 121.41      | 115.23   |
| 11  | M     | 400    | BCB  | O2D-CGD-CBD | 3.55  | 117.43      | 111.23   |
| 11  | M     | 400    | BCB  | C2D-C1D-ND  | -3.52 | 106.65      | 110.13   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | L     | 400 | BCB  | C4-C3-C5    | 3.51  | 121.33      | 115.23   |
| 16  | M     | 600 | NS5  | C13-C12-C10 | -3.51 | 122.76      | 127.69   |
| 13  | L     | 502 | UQ9  | C35-C34-C36 | 3.42  | 121.16      | 115.23   |
| 9   | M     | 333 | HTO  | O1-C1-C2    | -3.42 | 103.98      | 111.16   |
| 11  | L     | 400 | BCB  | C3C-C4C-NC  | 3.41  | 114.67      | 110.45   |
| 13  | L     | 502 | UQ9  | C1M-C1-C6   | -3.40 | 118.86      | 124.45   |
| 11  | M     | 401 | BCB  | CED-O2D-CGD | 3.37  | 123.55      | 115.92   |
| 12  | M     | 402 | BPB  | C2D-C1D-ND  | -3.30 | 107.04      | 109.43   |
| 5   | C     | 404 | HEC  | CMD-C2D-C1D | 3.27  | 130.14      | 125.03   |
| 11  | M     | 400 | BCB  | C4-C3-C5    | 3.26  | 120.89      | 115.23   |
| 11  | M     | 401 | BCB  | O2A-CGA-CBA | 3.24  | 121.71      | 111.83   |
| 5   | C     | 404 | HEC  | C3B-C4B-NB  | 3.23  | 113.72      | 110.17   |
| 11  | L     | 400 | BCB  | C2D-C1D-ND  | -3.23 | 106.93      | 110.13   |
| 5   | C     | 403 | HEC  | CHD-C1D-ND  | -3.21 | 120.40      | 124.37   |
| 11  | M     | 401 | BCB  | CMD-C2D-C1D | 3.20  | 130.36      | 124.73   |
| 13  | L     | 503 | UQ9  | C1-C6-C5    | -3.16 | 116.55      | 119.62   |
| 15  | M     | 501 | MQ9  | C40-C39-C38 | -3.16 | 115.52      | 123.63   |
| 11  | M     | 401 | BCB  | C2D-C1D-ND  | -3.13 | 107.02      | 110.13   |
| 6   | L     | 708 | LDA  | CM1-N1-C1   | -3.13 | 103.65      | 110.23   |
| 5   | C     | 401 | HEC  | CHC-C4B-NB  | -3.13 | 120.50      | 124.37   |
| 6   | M     | 704 | LDA  | CM2-N1-C1   | 3.12  | 116.78      | 110.23   |
| 5   | C     | 404 | HEC  | C3C-C4C-NC  | 3.12  | 113.61      | 110.15   |
| 7   | C     | 730 | DGA  | OG1-CA1-CA2 | 3.11  | 121.33      | 111.83   |
| 15  | M     | 501 | MQ9  | C5M-C5-C6   | -3.11 | 119.34      | 124.45   |
| 9   | H     | 272 | HTO  | C5-C4-C3    | -3.09 | 109.05      | 114.11   |
| 12  | L     | 402 | BPB  | CED-O2D-CGD | 3.07  | 122.87      | 115.92   |
| 12  | M     | 402 | BPB  | O2D-CGD-CBD | 3.06  | 114.31      | 110.95   |
| 16  | M     | 600 | NS5  | C32-C31-C33 | 3.04  | 120.50      | 115.23   |
| 11  | M     | 400 | BCB  | CBA-CAA-C2A | -3.02 | 104.82      | 113.79   |
| 13  | L     | 502 | UQ9  | C7-C8-C9    | 3.01  | 132.01      | 126.83   |
| 13  | L     | 502 | UQ9  | C7-C6-C5    | -3.01 | 115.02      | 118.52   |
| 11  | L     | 401 | BCB  | C6-C5-C3    | -2.99 | 106.18      | 113.47   |
| 11  | L     | 400 | BCB  | C1-C2-C3    | -2.99 | 121.30      | 126.20   |
| 11  | L     | 401 | BCB  | O2D-CGD-CBD | 2.96  | 116.41      | 111.23   |
| 15  | M     | 501 | MQ9  | C15-C14-C16 | 2.95  | 120.35      | 115.23   |
| 9   | L     | 278 | HTO  | O2-C2-C1    | -2.93 | 102.35      | 109.03   |
| 5   | C     | 401 | HEC  | C3B-C4B-NB  | 2.93  | 113.39      | 110.17   |
| 7   | C     | 730 | DGA  | OG2-CG2-CG1 | 2.92  | 112.93      | 106.21   |
| 11  | M     | 400 | BCB  | CMD-C2D-C1D | 2.89  | 129.82      | 124.73   |
| 12  | L     | 402 | BPB  | C3B-C4B-NB  | -2.87 | 103.88      | 108.05   |
| 9   | L     | 278 | HTO  | O1-C1-C2    | -2.86 | 105.16      | 111.16   |
| 12  | M     | 402 | BPB  | C2B-C1B-NB  | -2.86 | 107.37      | 109.43   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 9   | H     | 272    | HTO  | O1-C1-C2    | -2.85 | 105.16      | 111.16   |
| 12  | L     | 402    | BPB  | OBD-CAD-C3D | 2.84  | 132.32      | 127.89   |
| 11  | L     | 400    | BCB  | CHA-C4D-ND  | 2.82  | 138.37      | 132.55   |
| 12  | L     | 402    | BPB  | O2D-CGD-CBD | 2.81  | 114.04      | 110.95   |
| 15  | M     | 501    | MQ9  | C35-C34-C36 | 2.80  | 120.08      | 115.23   |
| 5   | C     | 403    | HEC  | C2D-C1D-ND  | 2.79  | 113.05      | 109.84   |
| 11  | M     | 401    | BCB  | CMD-C2D-C3D | -2.77 | 121.34      | 127.69   |
| 6   | L     | 708    | LDA  | O1-N1-C1    | 2.76  | 116.04      | 109.27   |
| 12  | M     | 402    | BPB  | CMD-C2D-C3D | 2.75  | 130.19      | 124.68   |
| 13  | L     | 502    | UQ9  | C6-C1-C2    | 2.75  | 121.34      | 119.17   |
| 5   | C     | 404    | HEC  | O2A-CGA-CBA | 2.75  | 122.69      | 114.00   |
| 5   | C     | 404    | HEC  | CHB-C1B-NB  | -2.75 | 121.47      | 124.42   |
| 17  | M     | 332    | HTH  | O3-C3-C2    | -2.74 | 103.81      | 109.57   |
| 5   | C     | 402    | HEC  | C3C-C4C-NC  | 2.74  | 113.20      | 110.15   |
| 5   | C     | 401    | HEC  | CMA-C3A-C4A | 2.73  | 129.53      | 124.73   |
| 5   | C     | 404    | HEC  | CHA-C1A-NA  | -2.70 | 121.51      | 124.45   |
| 11  | L     | 401    | BCB  | OBD-CAD-C3D | -2.70 | 122.10      | 128.42   |
| 12  | L     | 402    | BPB  | CMD-C2D-C3D | 2.66  | 130.00      | 124.68   |
| 11  | L     | 400    | BCB  | O2A-CGA-CBA | 2.66  | 119.93      | 111.83   |
| 11  | M     | 400    | BCB  | CHC-C1C-NC  | -2.64 | 120.58      | 124.40   |
| 9   | C     | 358[A] | HTO  | O2-C2-C1    | -2.63 | 103.06      | 109.03   |
| 5   | C     | 401    | HEC  | CAD-C3D-C4D | 2.62  | 129.26      | 124.70   |
| 11  | L     | 400    | BCB  | CMD-C2D-C3D | -2.61 | 121.70      | 127.69   |
| 5   | C     | 404    | HEC  | O1D-CGD-CBD | -2.60 | 114.85      | 123.09   |
| 5   | C     | 401    | HEC  | CBB-CAB-C3B | -2.57 | 105.45      | 112.42   |
| 5   | C     | 402    | HEC  | CHC-C4B-NB  | -2.56 | 121.20      | 124.37   |
| 13  | L     | 502    | UQ9  | C45-C44-C46 | 2.55  | 119.66      | 115.23   |
| 13  | L     | 502    | UQ9  | C1-C6-C5    | -2.55 | 117.14      | 119.62   |
| 11  | L     | 401    | BCB  | O1D-CGD-CBD | -2.55 | 119.49      | 124.52   |
| 5   | C     | 404    | HEC  | C2D-C1D-ND  | 2.54  | 112.76      | 109.84   |
| 15  | M     | 501    | MQ9  | C25-C24-C26 | 2.53  | 119.62      | 115.23   |
| 11  | L     | 401    | BCB  | C3D-C4D-ND  | -2.53 | 105.88      | 109.99   |
| 5   | C     | 401    | HEC  | CMC-C2C-C3C | 2.52  | 130.97      | 125.62   |
| 11  | M     | 400    | BCB  | O2A-CGA-CBA | 2.52  | 119.52      | 111.83   |
| 11  | M     | 401    | BCB  | CAA-C2A-C3A | -2.52 | 106.20      | 113.00   |
| 5   | C     | 404    | HEC  | C1D-C2D-C3D | -2.50 | 104.35      | 106.98   |
| 5   | C     | 401    | HEC  | CHA-C4D-ND  | -2.50 | 121.73      | 124.42   |
| 5   | C     | 402    | HEC  | C2D-C1D-ND  | 2.47  | 112.67      | 109.84   |
| 11  | M     | 401    | BCB  | CHA-C4D-ND  | 2.46  | 137.63      | 132.55   |
| 5   | C     | 404    | HEC  | C3D-C4D-ND  | 2.46  | 112.73      | 110.35   |
| 5   | C     | 403    | HEC  | C3C-C4C-NC  | 2.46  | 112.88      | 110.15   |
| 9   | C     | 355    | HTO  | O2-C2-C1    | 2.46  | 114.61      | 109.03   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | C     | 401 | HEC  | C2D-C1D-ND  | 2.45  | 112.66      | 109.84   |
| 13  | L     | 503 | UQ9  | C8-C7-C6    | -2.45 | 106.05      | 112.08   |
| 9   | L     | 276 | HTO  | O2-C2-C3    | -2.43 | 104.47      | 109.57   |
| 13  | L     | 502 | UQ9  | O5-C5-C6    | -2.41 | 117.12      | 121.79   |
| 12  | L     | 402 | BPB  | CMB-C2B-C3B | 2.41  | 129.51      | 124.68   |
| 9   | L     | 278 | HTO  | O2-C2-C3    | 2.41  | 114.64      | 109.57   |
| 5   | C     | 402 | HEC  | CAA-C2A-C1A | 2.40  | 129.74      | 124.85   |
| 15  | M     | 501 | MQ9  | C40-C39-C41 | 2.40  | 119.40      | 115.23   |
| 5   | C     | 404 | HEC  | C4B-C3B-C2B | -2.40 | 103.40      | 106.89   |
| 5   | C     | 402 | HEC  | C1A-C2A-C3A | -2.40 | 103.95      | 107.11   |
| 5   | C     | 404 | HEC  | CAB-C3B-C4B | 2.36  | 127.87      | 124.79   |
| 16  | M     | 600 | NS5  | C24-C23-C21 | -2.35 | 119.92      | 126.36   |
| 16  | M     | 600 | NS5  | C27-C26-C28 | 2.35  | 121.68      | 118.09   |
| 13  | L     | 502 | UQ9  | O2-C2-C3    | -2.33 | 116.10      | 121.03   |
| 9   | L     | 276 | HTO  | O3-C3-C4    | 2.32  | 114.41      | 109.14   |
| 9   | H     | 272 | HTO  | O2-C2-C1    | -2.32 | 103.76      | 109.03   |
| 15  | M     | 501 | MQ9  | C3D-C2-C3   | 2.31  | 121.86      | 119.26   |
| 12  | L     | 402 | BPB  | C1-C2-C3    | -2.31 | 122.42      | 126.20   |
| 12  | M     | 402 | BPB  | C1-O2A-CGA  | 2.31  | 122.24      | 116.65   |
| 11  | M     | 401 | BCB  | C2B-C1B-NB  | 2.30  | 112.71      | 110.33   |
| 11  | M     | 401 | BCB  | C1C-NC-C4C  | -2.28 | 105.64      | 106.68   |
| 11  | M     | 401 | BCB  | C3C-C4C-NC  | 2.28  | 113.27      | 110.45   |
| 13  | L     | 502 | UQ9  | C45-C44-C43 | -2.27 | 117.79      | 123.63   |
| 11  | M     | 401 | BCB  | C4-C3-C5    | 2.27  | 119.17      | 115.23   |
| 11  | L     | 401 | BCB  | CMB-C2B-C3B | 2.27  | 132.83      | 125.67   |
| 5   | C     | 401 | HEC  | CHB-C1B-NB  | -2.27 | 121.98      | 124.42   |
| 6   | M     | 704 | LDA  | O1-N1-C1    | 2.25  | 114.80      | 109.27   |
| 11  | L     | 401 | BCB  | CHD-C4C-NC  | -2.25 | 120.74      | 124.23   |
| 5   | C     | 403 | HEC  | C3D-C4D-ND  | 2.25  | 112.52      | 110.35   |
| 5   | C     | 403 | HEC  | CHA-C4D-ND  | -2.24 | 122.01      | 124.42   |
| 12  | M     | 402 | BPB  | C3D-CAD-CBD | 2.24  | 110.56      | 107.61   |
| 13  | L     | 503 | UQ9  | C3-C2-C1    | 2.24  | 122.53      | 118.10   |
| 9   | H     | 273 | HTO  | O1-C1-C2    | 2.24  | 115.85      | 111.16   |
| 11  | L     | 400 | BCB  | C5-C3-C2    | -2.23 | 116.17      | 121.17   |
| 11  | L     | 400 | BCB  | O2D-CGD-O1D | -2.22 | 119.53      | 123.85   |
| 5   | C     | 404 | HEC  | C2B-C1B-NB  | 2.22  | 112.46      | 109.90   |
| 9   | L     | 280 | HTO  | C5-C4-C3    | -2.21 | 110.49      | 114.11   |
| 9   | C     | 356 | HTO  | C5-C4-C3    | 2.21  | 117.73      | 114.11   |
| 5   | C     | 401 | HEC  | C4C-C3C-C2C | -2.20 | 103.46      | 106.87   |
| 5   | C     | 404 | HEC  | O2D-CGD-CBD | 2.20  | 120.96      | 114.00   |
| 10  | L     | 282 | GOL  | C3-C2-C1    | 2.20  | 119.86      | 111.80   |
| 5   | C     | 404 | HEC  | CHA-C4D-ND  | -2.20 | 122.06      | 124.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | C     | 402 | HEC  | CMC-C2C-C3C | 2.20  | 130.28      | 125.62   |
| 5   | C     | 403 | HEC  | C4C-CHD-C1D | 2.19  | 131.39      | 126.25   |
| 11  | M     | 400 | BCB  | CHD-C4C-C3C | -2.18 | 123.18      | 125.91   |
| 11  | L     | 401 | BCB  | C1-C2-C3    | -2.18 | 122.63      | 126.20   |
| 5   | C     | 401 | HEC  | CHD-C4C-NC  | -2.17 | 119.92      | 123.86   |
| 11  | L     | 401 | BCB  | C5-C3-C2    | -2.16 | 116.32      | 121.17   |
| 11  | L     | 400 | BCB  | CMA-C3A-C4A | 2.16  | 117.57      | 111.77   |
| 9   | M     | 333 | HTO  | O3-C3-C2    | 2.16  | 114.11      | 109.57   |
| 9   | C     | 355 | HTO  | C4-C3-C2    | -2.15 | 108.56      | 113.73   |
| 16  | M     | 600 | NS5  | C28-C26-C25 | -2.14 | 115.64      | 119.01   |
| 5   | C     | 404 | HEC  | O2A-CGA-O1A | -2.13 | 117.85      | 123.33   |
| 11  | M     | 401 | BCB  | CHC-C1C-NC  | -2.13 | 121.33      | 124.40   |
| 13  | L     | 502 | UQ9  | C15-C14-C16 | 2.13  | 118.92      | 115.23   |
| 13  | L     | 503 | UQ9  | C15-C14-C16 | 2.12  | 119.47      | 114.59   |
| 5   | C     | 402 | HEC  | CAB-C3B-C4B | 2.12  | 127.55      | 124.79   |
| 9   | M     | 333 | HTO  | O3-C3-C4    | -2.11 | 104.34      | 109.14   |
| 10  | C     | 361 | GOL  | O1-C1-C2    | -2.11 | 100.90      | 110.38   |
| 5   | C     | 401 | HEC  | C4C-NC-C1C  | -2.10 | 102.39      | 105.82   |
| 5   | C     | 401 | HEC  | O2A-CGA-CBA | 2.10  | 120.64      | 114.00   |
| 5   | C     | 403 | HEC  | C4A-C3A-C2A | -2.10 | 103.86      | 106.97   |
| 11  | M     | 400 | BCB  | C3D-C4D-ND  | -2.10 | 106.58      | 109.99   |
| 11  | M     | 401 | BCB  | CMA-C3A-C4A | 2.10  | 117.40      | 111.77   |
| 11  | M     | 401 | BCB  | CAA-CBA-CGA | -2.09 | 107.26      | 113.21   |
| 7   | C     | 730 | DGA  | OG1-CA1-OA1 | -2.08 | 118.42      | 123.63   |
| 7   | C     | 730 | DGA  | OG1-CG1-CG2 | 2.08  | 114.27      | 108.35   |
| 5   | C     | 402 | HEC  | CHB-C1B-NB  | -2.07 | 122.19      | 124.42   |
| 5   | C     | 403 | HEC  | C2C-C1C-NC  | 2.06  | 113.45      | 110.14   |
| 10  | H     | 280 | GOL  | C3-C2-C1    | 2.06  | 119.34      | 111.80   |
| 11  | M     | 400 | BCB  | O1D-CGD-CBD | -2.05 | 120.47      | 124.52   |
| 9   | L     | 279 | HTO  | C4-C3-C2    | -2.05 | 108.81      | 113.73   |
| 5   | C     | 402 | HEC  | C2A-C1A-NA  | 2.04  | 112.29      | 110.32   |
| 15  | M     | 501 | MQ9  | C51-C49-C50 | 2.03  | 119.27      | 114.59   |
| 5   | C     | 403 | HEC  | O2A-CGA-O1A | -2.03 | 118.12      | 123.33   |
| 5   | C     | 404 | HEC  | CHC-C4B-NB  | -2.02 | 121.87      | 124.37   |
| 13  | L     | 502 | UQ9  | C25-C24-C23 | -2.01 | 118.46      | 123.63   |
| 12  | L     | 402 | BPB  | O2A-CGA-O1A | -2.01 | 118.60      | 123.63   |
| 9   | C     | 355 | HTO  | C1-C2-C3    | -2.01 | 108.91      | 113.00   |
| 11  | L     | 401 | BCB  | CMD-C2D-C1D | 2.01  | 128.27      | 124.73   |
| 9   | H     | 272 | HTO  | C1-C2-C3    | 2.01  | 117.09      | 113.00   |

All (16) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 5   | C     | 401 | HEC  | NA   |
| 5   | C     | 402 | HEC  | NA   |
| 5   | C     | 403 | HEC  | NA   |
| 5   | C     | 404 | HEC  | NA   |
| 11  | L     | 400 | BCB  | NC   |
| 11  | L     | 400 | BCB  | ND   |
| 11  | L     | 400 | BCB  | NA   |
| 11  | L     | 401 | BCB  | NC   |
| 11  | L     | 401 | BCB  | ND   |
| 11  | L     | 401 | BCB  | NA   |
| 11  | M     | 400 | BCB  | NC   |
| 11  | M     | 400 | BCB  | ND   |
| 11  | M     | 400 | BCB  | NA   |
| 11  | M     | 401 | BCB  | NC   |
| 11  | M     | 401 | BCB  | ND   |
| 11  | M     | 401 | BCB  | NA   |

All (474) torsion outliers are listed below:

| Mol | Chain | Res    | Type | Atoms        |
|-----|-------|--------|------|--------------|
| 6   | C     | 716    | LDA  | C2-C1-N1-CM1 |
| 6   | C     | 716    | LDA  | N1-C1-C2-C3  |
| 6   | C     | 722    | LDA  | C2-C1-N1-O1  |
| 6   | C     | 722    | LDA  | N1-C1-C2-C3  |
| 6   | H     | 718[B] | LDA  | C2-C1-N1-O1  |
| 6   | H     | 718[B] | LDA  | C2-C1-N1-CM1 |
| 6   | H     | 718[B] | LDA  | C2-C1-N1-CM2 |
| 6   | H     | 721    | LDA  | C2-C1-N1-CM1 |
| 6   | H     | 721    | LDA  | C2-C1-N1-CM2 |
| 6   | L     | 702    | LDA  | C2-C1-N1-CM1 |
| 6   | L     | 703    | LDA  | N1-C1-C2-C3  |
| 6   | L     | 710    | LDA  | C2-C1-N1-CM1 |
| 6   | L     | 710    | LDA  | C2-C1-N1-CM2 |
| 6   | L     | 712    | LDA  | N1-C1-C2-C3  |
| 6   | L     | 723    | LDA  | C2-C1-N1-O1  |
| 6   | L     | 723    | LDA  | C2-C1-N1-CM2 |
| 6   | L     | 724    | LDA  | C2-C1-N1-CM1 |
| 6   | M     | 706    | LDA  | C2-C1-N1-CM1 |
| 6   | M     | 706    | LDA  | C2-C1-N1-CM2 |
| 6   | M     | 707    | LDA  | C2-C1-N1-CM1 |
| 6   | M     | 707    | LDA  | C2-C1-N1-CM2 |
| 6   | M     | 707    | LDA  | N1-C1-C2-C3  |
| 6   | M     | 714    | LDA  | N1-C1-C2-C3  |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 7   | C     | 730    | DGA  | CB2-CB1-OG2-CG2 |
| 7   | C     | 730    | DGA  | OB1-CB1-OG2-CG2 |
| 7   | C     | 730    | DGA  | OG1-CG1-CG2-OG2 |
| 7   | C     | 730    | DGA  | CG1-CG2-OG2-CB1 |
| 9   | C     | 355    | HTO  | O3-C3-C4-C5     |
| 9   | C     | 356    | HTO  | C1-C2-C3-O3     |
| 9   | C     | 356    | HTO  | C1-C2-C3-C4     |
| 9   | C     | 356    | HTO  | O2-C2-C3-O3     |
| 9   | C     | 356    | HTO  | O2-C2-C3-C4     |
| 9   | C     | 356    | HTO  | O3-C3-C4-C5     |
| 9   | C     | 357    | HTO  | C1-C2-C3-C4     |
| 9   | C     | 357    | HTO  | O2-C2-C3-C4     |
| 9   | C     | 358[A] | HTO  | C1-C2-C3-O3     |
| 9   | C     | 358[A] | HTO  | C1-C2-C3-C4     |
| 9   | C     | 358[A] | HTO  | O2-C2-C3-O3     |
| 9   | C     | 358[A] | HTO  | O2-C2-C3-C4     |
| 9   | C     | 358[A] | HTO  | O3-C3-C4-C5     |
| 9   | H     | 274[A] | HTO  | O1-C1-C2-O2     |
| 9   | H     | 274[A] | HTO  | O1-C1-C2-C3     |
| 9   | H     | 274[A] | HTO  | C2-C3-C4-C5     |
| 9   | H     | 274[A] | HTO  | O3-C3-C4-C5     |
| 9   | L     | 276    | HTO  | C1-C2-C3-O3     |
| 9   | L     | 276    | HTO  | C1-C2-C3-C4     |
| 9   | L     | 276    | HTO  | O2-C2-C3-O3     |
| 9   | L     | 276    | HTO  | O2-C2-C3-C4     |
| 9   | L     | 278    | HTO  | C1-C2-C3-O3     |
| 9   | L     | 278    | HTO  | O2-C2-C3-O3     |
| 9   | L     | 278    | HTO  | O2-C2-C3-C4     |
| 9   | L     | 279    | HTO  | O3-C3-C4-C5     |
| 9   | M     | 333    | HTO  | C1-C2-C3-O3     |
| 9   | M     | 333    | HTO  | C1-C2-C3-C4     |
| 9   | M     | 333    | HTO  | O2-C2-C3-O3     |
| 9   | M     | 333    | HTO  | O2-C2-C3-C4     |
| 9   | M     | 333    | HTO  | O3-C3-C4-C5     |
| 10  | C     | 362    | GOL  | C1-C2-C3-O3     |
| 10  | C     | 362    | GOL  | O2-C2-C3-O3     |
| 10  | C     | 364    | GOL  | O1-C1-C2-C3     |
| 10  | C     | 365    | GOL  | C1-C2-C3-O3     |
| 10  | C     | 366    | GOL  | O1-C1-C2-C3     |
| 10  | C     | 367    | GOL  | C1-C2-C3-O3     |
| 10  | C     | 368    | GOL  | O1-C1-C2-C3     |
| 10  | C     | 368    | GOL  | C1-C2-C3-O3     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 10  | C     | 373    | GOL  | O1-C1-C2-O2     |
| 10  | C     | 373    | GOL  | O1-C1-C2-C3     |
| 10  | C     | 374[B] | GOL  | O1-C1-C2-C3     |
| 10  | C     | 374[B] | GOL  | C1-C2-C3-O3     |
| 10  | H     | 275    | GOL  | C1-C2-C3-O3     |
| 10  | H     | 276[A] | GOL  | C1-C2-C3-O3     |
| 10  | H     | 278    | GOL  | C1-C2-C3-O3     |
| 10  | H     | 278    | GOL  | O2-C2-C3-O3     |
| 10  | H     | 280    | GOL  | C1-C2-C3-O3     |
| 10  | H     | 282    | GOL  | O1-C1-C2-C3     |
| 10  | H     | 283    | GOL  | O1-C1-C2-C3     |
| 10  | H     | 283    | GOL  | C1-C2-C3-O3     |
| 10  | H     | 284    | GOL  | O1-C1-C2-C3     |
| 10  | H     | 285    | GOL  | C1-C2-C3-O3     |
| 10  | H     | 286    | GOL  | C1-C2-C3-O3     |
| 10  | H     | 287    | GOL  | O1-C1-C2-C3     |
| 10  | H     | 287    | GOL  | C1-C2-C3-O3     |
| 10  | H     | 288    | GOL  | O1-C1-C2-C3     |
| 10  | H     | 289    | GOL  | O1-C1-C2-C3     |
| 10  | H     | 289    | GOL  | C1-C2-C3-O3     |
| 10  | H     | 290    | GOL  | C1-C2-C3-O3     |
| 10  | H     | 291    | GOL  | C1-C2-C3-O3     |
| 10  | L     | 282    | GOL  | O1-C1-C2-C3     |
| 10  | L     | 284    | GOL  | O1-C1-C2-C3     |
| 10  | L     | 284    | GOL  | C1-C2-C3-O3     |
| 10  | L     | 285    | GOL  | O1-C1-C2-C3     |
| 10  | L     | 286    | GOL  | O1-C1-C2-C3     |
| 10  | L     | 286    | GOL  | C1-C2-C3-O3     |
| 10  | L     | 288    | GOL  | C1-C2-C3-O3     |
| 10  | L     | 288    | GOL  | O2-C2-C3-O3     |
| 10  | M     | 334    | GOL  | C1-C2-C3-O3     |
| 10  | M     | 336    | GOL  | O1-C1-C2-C3     |
| 10  | M     | 336    | GOL  | C1-C2-C3-O3     |
| 10  | M     | 338    | GOL  | O1-C1-C2-C3     |
| 10  | M     | 338    | GOL  | C1-C2-C3-O3     |
| 10  | M     | 340    | GOL  | C1-C2-C3-O3     |
| 10  | M     | 342    | GOL  | O1-C1-C2-C3     |
| 10  | M     | 342    | GOL  | C1-C2-C3-O3     |
| 11  | L     | 400    | BCB  | C2C-C3C-CAC-CBC |
| 11  | M     | 400    | BCB  | C2C-C3C-CAC-CBC |
| 11  | M     | 401    | BCB  | C2C-C3C-CAC-CBC |
| 11  | M     | 401    | BCB  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 11  | M     | 401    | BCB  | CAD-CBD-CGD-O2D |
| 12  | L     | 402    | BPB  | C2C-C3C-CAC-CBC |
| 16  | M     | 600    | NS5  | C3-C4-C5-C6     |
| 17  | M     | 332    | HTH  | C1-C2-C3-O3     |
| 17  | M     | 332    | HTH  | O2-C2-C3-C4     |
| 16  | M     | 600    | NS5  | C3-C4-C5-C7     |
| 6   | H     | 720    | LDA  | C1-C2-C3-C4     |
| 9   | C     | 357    | HTO  | O1-C1-C2-O2     |
| 9   | C     | 358[A] | HTO  | O1-C1-C2-O2     |
| 9   | H     | 273    | HTO  | O1-C1-C2-O2     |
| 9   | C     | 357    | HTO  | O1-C1-C2-C3     |
| 9   | H     | 273    | HTO  | O1-C1-C2-C3     |
| 5   | C     | 401    | HEC  | C2B-C3B-CAB-CBB |
| 6   | L     | 723    | LDA  | C3-C4-C5-C6     |
| 5   | C     | 403    | HEC  | C2B-C3B-CAB-CBB |
| 11  | L     | 400    | BCB  | C4-C3-C5-C6     |
| 12  | M     | 402    | BPB  | C4-C3-C5-C6     |
| 11  | L     | 400    | BCB  | C2-C3-C5-C6     |
| 12  | M     | 402    | BPB  | C2-C3-C5-C6     |
| 16  | M     | 600    | NS5  | C12-C10-C9-C8   |
| 6   | H     | 720    | LDA  | C3-C4-C5-C6     |
| 13  | L     | 502    | UQ9  | C39-C41-C42-C43 |
| 13  | L     | 502    | UQ9  | C34-C36-C37-C38 |
| 11  | M     | 401    | BCB  | C2A-CAA-CBA-CGA |
| 6   | M     | 706    | LDA  | C3-C4-C5-C6     |
| 16  | M     | 600    | NS5  | C11-C10-C9-C8   |
| 6   | C     | 722    | LDA  | C3-C4-C5-C6     |
| 10  | C     | 368    | GOL  | O2-C2-C3-O3     |
| 10  | H     | 275    | GOL  | O2-C2-C3-O3     |
| 10  | H     | 287    | GOL  | O2-C2-C3-O3     |
| 10  | H     | 289    | GOL  | O2-C2-C3-O3     |
| 10  | L     | 285    | GOL  | O1-C1-C2-O2     |
| 12  | M     | 402    | BPB  | C11-C12-C13-C15 |
| 13  | L     | 502    | UQ9  | C24-C26-C27-C28 |
| 7   | C     | 730    | DGA  | CB1-CB2-CB3-CB4 |
| 11  | M     | 400    | BCB  | C8-C10-C11-C12  |
| 5   | C     | 403    | HEC  | C4B-C3B-CAB-CBB |
| 7   | C     | 730    | DGA  | CA1-CA2-CA3-CA4 |
| 11  | L     | 400    | BCB  | C15-C16-C17-C18 |
| 7   | C     | 730    | DGA  | CA2-CA1-OG1-CG1 |
| 9   | H     | 273    | HTO  | C2-C3-C4-C5     |
| 5   | C     | 401    | HEC  | C4C-C3C-CAC-CBC |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 5   | C     | 403    | HEC  | C4C-C3C-CAC-CBC |
| 13  | L     | 502    | UQ9  | C29-C31-C32-C33 |
| 6   | L     | 702    | LDA  | C2-C3-C4-C5     |
| 10  | C     | 369    | GOL  | C1-C2-C3-O3     |
| 10  | C     | 372    | GOL  | O1-C1-C2-C3     |
| 10  | C     | 376    | GOL  | O1-C1-C2-C3     |
| 10  | C     | 377    | GOL  | O1-C1-C2-C3     |
| 10  | C     | 378    | GOL  | O1-C1-C2-C3     |
| 10  | H     | 276[A] | GOL  | O1-C1-C2-C3     |
| 10  | H     | 276[B] | GOL  | O1-C1-C2-C3     |
| 10  | H     | 277    | GOL  | O1-C1-C2-C3     |
| 10  | L     | 283    | GOL  | C1-C2-C3-O3     |
| 10  | M     | 334    | GOL  | O1-C1-C2-C3     |
| 10  | M     | 337    | GOL  | O1-C1-C2-C3     |
| 10  | M     | 339    | GOL  | C1-C2-C3-O3     |
| 6   | L     | 703    | LDA  | C5-C6-C7-C8     |
| 9   | C     | 355    | HTO  | O1-C1-C2-O2     |
| 11  | L     | 401    | BCB  | C16-C17-C18-C19 |
| 6   | C     | 722    | LDA  | C6-C7-C8-C9     |
| 6   | M     | 714    | LDA  | C5-C6-C7-C8     |
| 7   | C     | 730    | DGA  | CB5-CB6-CB7-CB8 |
| 6   | L     | 710    | LDA  | C6-C7-C8-C9     |
| 6   | M     | 704    | LDA  | C2-C3-C4-C5     |
| 10  | C     | 364    | GOL  | O1-C1-C2-O2     |
| 10  | C     | 365    | GOL  | O2-C2-C3-O3     |
| 10  | C     | 366    | GOL  | O1-C1-C2-O2     |
| 10  | C     | 368    | GOL  | O1-C1-C2-O2     |
| 10  | C     | 372    | GOL  | O1-C1-C2-O2     |
| 10  | C     | 374[B] | GOL  | O1-C1-C2-O2     |
| 10  | C     | 374[B] | GOL  | O2-C2-C3-O3     |
| 10  | H     | 276[A] | GOL  | O1-C1-C2-O2     |
| 10  | H     | 276[A] | GOL  | O2-C2-C3-O3     |
| 10  | H     | 276[B] | GOL  | O1-C1-C2-O2     |
| 10  | H     | 282    | GOL  | O1-C1-C2-O2     |
| 10  | H     | 284    | GOL  | O1-C1-C2-O2     |
| 10  | H     | 285    | GOL  | O2-C2-C3-O3     |
| 10  | H     | 286    | GOL  | O2-C2-C3-O3     |
| 10  | H     | 287    | GOL  | O1-C1-C2-O2     |
| 10  | H     | 289    | GOL  | O1-C1-C2-O2     |
| 10  | H     | 290    | GOL  | O2-C2-C3-O3     |
| 10  | L     | 282    | GOL  | O1-C1-C2-O2     |
| 10  | L     | 284    | GOL  | O1-C1-C2-O2     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 10  | L     | 284    | GOL  | O2-C2-C3-O3     |
| 10  | M     | 334    | GOL  | O2-C2-C3-O3     |
| 10  | M     | 336    | GOL  | O2-C2-C3-O3     |
| 10  | M     | 340    | GOL  | O2-C2-C3-O3     |
| 10  | M     | 342    | GOL  | O2-C2-C3-O3     |
| 6   | H     | 721    | LDA  | C3-C4-C5-C6     |
| 6   | L     | 702    | LDA  | C4-C5-C6-C7     |
| 6   | M     | 704    | LDA  | C6-C7-C8-C9     |
| 7   | C     | 730    | DGA  | CA5-CA6-CA7-CA8 |
| 6   | L     | 712    | LDA  | C4-C5-C6-C7     |
| 6   | C     | 716    | LDA  | C3-C4-C5-C6     |
| 6   | M     | 705    | LDA  | C6-C7-C8-C9     |
| 6   | H     | 718[B] | LDA  | C4-C5-C6-C7     |
| 6   | L     | 724    | LDA  | C3-C4-C5-C6     |
| 7   | C     | 730    | DGA  | CB4-CB5-CB6-CB7 |
| 11  | M     | 401    | BCB  | C3A-C2A-CAA-CBA |
| 7   | C     | 730    | DGA  | CA4-CA5-CA6-CA7 |
| 6   | L     | 710    | LDA  | C4-C5-C6-C7     |
| 7   | C     | 730    | DGA  | OA1-CA1-OG1-CG1 |
| 6   | C     | 716    | LDA  | C6-C7-C8-C9     |
| 6   | H     | 721    | LDA  | C2-C3-C4-C5     |
| 6   | L     | 712    | LDA  | C2-C3-C4-C5     |
| 6   | L     | 712    | LDA  | C5-C6-C7-C8     |
| 6   | H     | 718[B] | LDA  | C3-C4-C5-C6     |
| 5   | C     | 403    | HEC  | C2C-C3C-CAC-CBC |
| 6   | L     | 703    | LDA  | C4-C5-C6-C7     |
| 6   | M     | 704    | LDA  | C5-C6-C7-C8     |
| 6   | M     | 713    | LDA  | C2-C3-C4-C5     |
| 6   | M     | 707    | LDA  | C4-C5-C6-C7     |
| 6   | M     | 705    | LDA  | C7-C8-C9-C10    |
| 7   | C     | 730    | DGA  | CB2-CB3-CB4-CB5 |
| 11  | M     | 400    | BCB  | C6-C7-C8-C9     |
| 6   | H     | 720    | LDA  | C4-C5-C6-C7     |
| 6   | L     | 710    | LDA  | C3-C4-C5-C6     |
| 6   | H     | 719    | LDA  | C2-C3-C4-C5     |
| 6   | L     | 702    | LDA  | C3-C4-C5-C6     |
| 6   | M     | 706    | LDA  | C5-C6-C7-C8     |
| 6   | M     | 714    | LDA  | C2-C3-C4-C5     |
| 6   | M     | 705    | LDA  | C11-C10-C9-C8   |
| 9   | C     | 355    | HTO  | C4-C5-C6-C7     |
| 6   | H     | 721    | LDA  | C4-C5-C6-C7     |
| 6   | H     | 718[B] | LDA  | C6-C7-C8-C9     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 13  | L     | 502    | UQ9  | C30-C29-C31-C32 |
| 6   | L     | 723    | LDA  | C1-C2-C3-C4     |
| 7   | C     | 730    | DGA  | CA2-CA3-CA4-CA5 |
| 13  | L     | 503    | UQ9  | C5-C6-C7-C8     |
| 6   | L     | 712    | LDA  | C7-C8-C9-C10    |
| 9   | C     | 356    | HTO  | O1-C1-C2-O2     |
| 6   | M     | 713    | LDA  | C11-C10-C9-C8   |
| 6   | M     | 715    | LDA  | C7-C8-C9-C10    |
| 13  | L     | 502    | UQ9  | C13-C14-C16-C17 |
| 6   | M     | 707    | LDA  | C1-C2-C3-C4     |
| 6   | L     | 708    | LDA  | C3-C4-C5-C6     |
| 5   | C     | 401    | HEC  | C4B-C3B-CAB-CBB |
| 10  | C     | 367    | GOL  | O2-C2-C3-O3     |
| 10  | C     | 376    | GOL  | O1-C1-C2-O2     |
| 10  | C     | 377    | GOL  | O1-C1-C2-O2     |
| 10  | H     | 280    | GOL  | O2-C2-C3-O3     |
| 10  | H     | 283    | GOL  | O1-C1-C2-O2     |
| 10  | H     | 288    | GOL  | O1-C1-C2-O2     |
| 10  | H     | 291    | GOL  | O2-C2-C3-O3     |
| 10  | L     | 286    | GOL  | O1-C1-C2-O2     |
| 10  | L     | 286    | GOL  | O2-C2-C3-O3     |
| 10  | M     | 338    | GOL  | O1-C1-C2-O2     |
| 10  | M     | 338    | GOL  | O2-C2-C3-O3     |
| 10  | M     | 342    | GOL  | O1-C1-C2-O2     |
| 6   | L     | 703    | LDA  | C7-C8-C9-C10    |
| 11  | M     | 401    | BCB  | C11-C12-C13-C15 |
| 12  | M     | 402    | BPB  | C11-C10-C8-C7   |
| 5   | C     | 404    | HEC  | C2B-C3B-CAB-CBB |
| 13  | L     | 502    | UQ9  | C28-C29-C31-C32 |
| 5   | C     | 401    | HEC  | C2C-C3C-CAC-CBC |
| 6   | H     | 721    | LDA  | C7-C8-C9-C10    |
| 6   | H     | 701    | LDA  | C4-C5-C6-C7     |
| 6   | M     | 705    | LDA  | C4-C5-C6-C7     |
| 6   | H     | 718[B] | LDA  | C7-C8-C9-C10    |
| 6   | L     | 724    | LDA  | C2-C3-C4-C5     |
| 6   | M     | 717    | LDA  | C4-C5-C6-C7     |
| 6   | L     | 724    | LDA  | C1-C2-C3-C4     |
| 9   | C     | 357    | HTO  | O2-C2-C3-O3     |
| 17  | M     | 332    | HTH  | O2-C2-C3-O3     |
| 6   | L     | 702    | LDA  | C11-C10-C9-C8   |
| 13  | L     | 502    | UQ9  | C15-C14-C16-C17 |
| 7   | C     | 730    | DGA  | CA7-CA8-CA9-CAA |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 12  | L     | 402    | BPB  | C8-C10-C11-C12  |
| 6   | L     | 711    | LDA  | C2-C3-C4-C5     |
| 12  | L     | 402    | BPB  | O2A-C1-C2-C3    |
| 6   | L     | 703    | LDA  | C6-C7-C8-C9     |
| 9   | M     | 333    | HTO  | C4-C5-C6-C7     |
| 6   | M     | 715    | LDA  | C5-C6-C7-C8     |
| 7   | C     | 730    | DGA  | CB6-CB7-CB8-CB9 |
| 6   | L     | 708    | LDA  | N1-C1-C2-C3     |
| 6   | L     | 723    | LDA  | N1-C1-C2-C3     |
| 6   | M     | 715    | LDA  | N1-C1-C2-C3     |
| 7   | C     | 730    | DGA  | CDB-CEB-CFB-CGB |
| 6   | L     | 724    | LDA  | C9-C10-C11-C12  |
| 5   | C     | 402    | HEC  | C4B-C3B-CAB-CBB |
| 9   | C     | 358[A] | HTO  | C4-C5-C6-C7     |
| 7   | C     | 730    | DGA  | CB7-CB8-CB9-CAB |
| 6   | C     | 716    | LDA  | C9-C10-C11-C12  |
| 6   | L     | 710    | LDA  | C9-C10-C11-C12  |
| 6   | M     | 714    | LDA  | C3-C4-C5-C6     |
| 6   | L     | 724    | LDA  | C11-C10-C9-C8   |
| 10  | C     | 364    | GOL  | O2-C2-C3-O3     |
| 10  | C     | 369    | GOL  | O2-C2-C3-O3     |
| 10  | C     | 378    | GOL  | O1-C1-C2-O2     |
| 10  | H     | 281    | GOL  | O1-C1-C2-O2     |
| 10  | H     | 283    | GOL  | O2-C2-C3-O3     |
| 10  | M     | 339    | GOL  | O2-C2-C3-O3     |
| 12  | M     | 402    | BPB  | C11-C10-C8-C9   |
| 5   | C     | 402    | HEC  | C2B-C3B-CAB-CBB |
| 11  | L     | 401    | BCB  | C12-C13-C15-C16 |
| 11  | M     | 400    | BCB  | C11-C10-C8-C7   |
| 9   | L     | 279    | HTO  | C4-C5-C6-C7     |
| 5   | C     | 404    | HEC  | C2C-C3C-CAC-CBC |
| 6   | L     | 712    | LDA  | C9-C10-C11-C12  |
| 6   | M     | 714    | LDA  | C9-C10-C11-C12  |
| 17  | M     | 332    | HTH  | O3-C3-C4-C5     |
| 17  | M     | 332    | HTH  | C4-C5-C6-C7     |
| 6   | L     | 709    | LDA  | C1-C2-C3-C4     |
| 7   | C     | 730    | DGA  | OG1-CG1-CG2-CG3 |
| 9   | C     | 358[A] | HTO  | O1-C1-C2-C3     |
| 6   | L     | 709    | LDA  | C7-C8-C9-C10    |
| 6   | M     | 705    | LDA  | C3-C4-C5-C6     |
| 6   | L     | 702    | LDA  | C5-C6-C7-C8     |
| 6   | H     | 701    | LDA  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | M     | 717 | LDA  | C7-C8-C9-C10    |
| 6   | H     | 719 | LDA  | C1-C2-C3-C4     |
| 6   | M     | 705 | LDA  | C2-C3-C4-C5     |
| 7   | C     | 730 | DGA  | CA3-CA4-CA5-CA6 |
| 7   | C     | 730 | DGA  | CEB-CFB-CGB-CHB |
| 9   | L     | 280 | HTO  | C2-C3-C4-C5     |
| 9   | L     | 280 | HTO  | C4-C5-C6-C7     |
| 6   | M     | 706 | LDA  | C9-C10-C11-C12  |
| 11  | M     | 400 | BCB  | C11-C10-C8-C9   |
| 6   | H     | 701 | LDA  | C7-C8-C9-C10    |
| 11  | L     | 401 | BCB  | C16-C17-C18-C20 |
| 10  | C     | 359 | GOL  | O1-C1-C2-O2     |
| 10  | C     | 370 | GOL  | O2-C2-C3-O3     |
| 10  | H     | 285 | GOL  | O1-C1-C2-O2     |
| 10  | M     | 334 | GOL  | O1-C1-C2-O2     |
| 10  | M     | 336 | GOL  | O1-C1-C2-O2     |
| 11  | M     | 400 | BCB  | C10-C11-C12-C13 |
| 6   | M     | 714 | LDA  | C7-C8-C9-C10    |
| 6   | H     | 721 | LDA  | C11-C10-C9-C8   |
| 6   | M     | 706 | LDA  | C6-C7-C8-C9     |
| 7   | C     | 730 | DGA  | CAB-CBB-CCB-CDB |
| 5   | C     | 402 | HEC  | C3D-CAD-CBD-CGD |
| 13  | L     | 503 | UQ9  | C1-C6-C7-C8     |
| 12  | M     | 402 | BPB  | C16-C17-C18-C20 |
| 15  | M     | 501 | MQ9  | C35-C34-C36-C37 |
| 6   | L     | 709 | LDA  | C5-C6-C7-C8     |
| 11  | M     | 400 | BCB  | C4-C3-C5-C6     |
| 15  | M     | 501 | MQ9  | C33-C34-C36-C37 |
| 6   | L     | 711 | LDA  | C7-C8-C9-C10    |
| 5   | C     | 404 | HEC  | C4B-C3B-CAB-CBB |
| 6   | C     | 716 | LDA  | C1-C2-C3-C4     |
| 11  | M     | 401 | BCB  | C11-C12-C13-C14 |
| 12  | M     | 402 | BPB  | C11-C12-C13-C14 |
| 6   | L     | 712 | LDA  | C3-C4-C5-C6     |
| 7   | C     | 730 | DGA  | CB3-CB4-CB5-CB6 |
| 6   | L     | 703 | LDA  | C1-C2-C3-C4     |
| 6   | H     | 720 | LDA  | C6-C7-C8-C9     |
| 6   | C     | 716 | LDA  | C2-C1-N1-CM2    |
| 6   | C     | 722 | LDA  | C2-C1-N1-CM2    |
| 6   | H     | 719 | LDA  | C2-C1-N1-CM1    |
| 6   | H     | 719 | LDA  | C2-C1-N1-CM2    |
| 6   | L     | 708 | LDA  | C2-C1-N1-CM1    |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 6   | L     | 708    | LDA  | C2-C1-N1-CM2    |
| 6   | M     | 704    | LDA  | C2-C1-N1-CM2    |
| 9   | L     | 280    | HTO  | O3-C3-C4-C5     |
| 6   | H     | 721    | LDA  | C9-C10-C11-C12  |
| 6   | L     | 723    | LDA  | C5-C6-C7-C8     |
| 16  | M     | 600    | NS5  | C31-C33-C34-C35 |
| 11  | M     | 401    | BCB  | C1A-C2A-CAA-CBA |
| 17  | M     | 332    | HTH  | C3-C4-C5-C6     |
| 6   | C     | 722    | LDA  | C2-C3-C4-C5     |
| 11  | M     | 400    | BCB  | C16-C17-C18-C19 |
| 11  | M     | 400    | BCB  | C16-C17-C18-C20 |
| 6   | M     | 713    | LDA  | C1-C2-C3-C4     |
| 16  | M     | 600    | NS5  | C17-C18-C19-C20 |
| 11  | L     | 401    | BCB  | C14-C13-C15-C16 |
| 6   | M     | 714    | LDA  | C6-C7-C8-C9     |
| 6   | C     | 716    | LDA  | C2-C1-N1-O1     |
| 6   | H     | 719    | LDA  | C2-C1-N1-O1     |
| 6   | L     | 708    | LDA  | C2-C1-N1-O1     |
| 6   | L     | 710    | LDA  | C2-C1-N1-O1     |
| 11  | M     | 400    | BCB  | C15-C16-C17-C18 |
| 6   | H     | 720    | LDA  | C7-C8-C9-C10    |
| 11  | M     | 400    | BCB  | C2-C3-C5-C6     |
| 11  | L     | 400    | BCB  | CAD-CBD-CGD-O2D |
| 6   | L     | 709    | LDA  | C4-C5-C6-C7     |
| 11  | L     | 400    | BCB  | CAD-CBD-CGD-O1D |
| 6   | L     | 710    | LDA  | C7-C8-C9-C10    |
| 6   | H     | 701    | LDA  | C9-C10-C11-C12  |
| 6   | C     | 722    | LDA  | C1-C2-C3-C4     |
| 11  | L     | 400    | BCB  | C16-C17-C18-C20 |
| 6   | H     | 720    | LDA  | C5-C6-C7-C8     |
| 6   | H     | 719    | LDA  | C3-C4-C5-C6     |
| 12  | M     | 402    | BPB  | C16-C17-C18-C19 |
| 11  | M     | 401    | BCB  | C3-C5-C6-C7     |
| 6   | M     | 704    | LDA  | C11-C10-C9-C8   |
| 13  | L     | 502    | UQ9  | C5-C4-O4-C4M    |
| 16  | M     | 600    | NS5  | C33-C34-C35-C36 |
| 6   | H     | 718[B] | LDA  | C11-C10-C9-C8   |
| 6   | L     | 709    | LDA  | N1-C1-C2-C3     |
| 6   | L     | 711    | LDA  | N1-C1-C2-C3     |
| 6   | M     | 707    | LDA  | C6-C7-C8-C9     |
| 6   | L     | 711    | LDA  | C5-C6-C7-C8     |
| 6   | L     | 708    | LDA  | C11-C10-C9-C8   |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 9   | C     | 358[A] | HTO  | C2-C3-C4-C5     |
| 10  | H     | 286    | GOL  | O1-C1-C2-O2     |
| 9   | C     | 356    | HTO  | C3-C4-C5-C6     |
| 9   | H     | 272    | HTO  | C3-C4-C5-C6     |
| 9   | L     | 278    | HTO  | C4-C5-C6-C7     |
| 6   | C     | 716    | LDA  | C4-C5-C6-C7     |
| 6   | M     | 706    | LDA  | C7-C8-C9-C10    |
| 9   | L     | 280    | HTO  | C3-C4-C5-C6     |
| 13  | L     | 503    | UQ9  | C2-C3-O3-C3M    |
| 6   | C     | 722    | LDA  | C4-C5-C6-C7     |
| 10  | C     | 370    | GOL  | C1-C2-C3-O3     |
| 6   | H     | 719    | LDA  | C9-C10-C11-C12  |
| 6   | C     | 716    | LDA  | C2-C3-C4-C5     |
| 5   | C     | 402    | HEC  | C2C-C3C-CAC-CBC |
| 5   | C     | 402    | HEC  | CAA-CBA-CGA-O1A |
| 5   | C     | 402    | HEC  | CAA-CBA-CGA-O2A |
| 7   | C     | 730    | DGA  | CA6-CA7-CA8-CA9 |
| 9   | L     | 280    | HTO  | O1-C1-C2-O2     |
| 13  | L     | 502    | UQ9  | C3-C4-O4-C4M    |
| 6   | L     | 723    | LDA  | C4-C5-C6-C7     |
| 6   | L     | 702    | LDA  | C6-C7-C8-C9     |
| 13  | L     | 502    | UQ9  | C40-C39-C41-C42 |
| 16  | M     | 600    | NS5  | C32-C31-C33-C34 |
| 5   | C     | 402    | HEC  | C4C-C3C-CAC-CBC |
| 7   | C     | 730    | DGA  | CA8-CA9-CAA-CBA |
| 6   | L     | 708    | LDA  | C2-C3-C4-C5     |
| 10  | C     | 367    | GOL  | O1-C1-C2-O2     |
| 10  | H     | 277    | GOL  | O1-C1-C2-O2     |
| 10  | L     | 283    | GOL  | O2-C2-C3-O3     |
| 10  | M     | 337    | GOL  | O1-C1-C2-O2     |
| 6   | M     | 706    | LDA  | C4-C5-C6-C7     |
| 9   | H     | 273    | HTO  | O3-C3-C4-C5     |
| 13  | L     | 502    | UQ9  | C4-C3-O3-C3M    |
| 6   | L     | 708    | LDA  | C5-C6-C7-C8     |
| 6   | L     | 723    | LDA  | C11-C10-C9-C8   |
| 5   | C     | 401    | HEC  | CAA-CBA-CGA-O2A |
| 9   | C     | 356    | HTO  | O1-C1-C2-C3     |
| 13  | L     | 502    | UQ9  | C46-C47-C48-C49 |
| 6   | M     | 715    | LDA  | C1-C2-C3-C4     |
| 5   | C     | 401    | HEC  | CAA-CBA-CGA-O1A |
| 7   | C     | 730    | DGA  | CA9-CAA-CBA-CCA |
| 9   | L     | 276    | HTO  | C3-C4-C5-C6     |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 10  | H     | 281    | GOL  | O2-C2-C3-O3     |
| 17  | M     | 332    | HTH  | C2-C3-C4-C5     |
| 6   | L     | 709    | LDA  | C11-C10-C9-C8   |
| 5   | C     | 404    | HEC  | C4C-C3C-CAC-CBC |
| 13  | L     | 502    | UQ9  | C20-C19-C21-C22 |
| 5   | C     | 402    | HEC  | CAD-CBD-CGD-O1D |
| 9   | C     | 358[A] | HTO  | C3-C4-C5-C6     |
| 9   | L     | 276    | HTO  | C4-C5-C6-C7     |
| 6   | C     | 722    | LDA  | C5-C6-C7-C8     |
| 6   | M     | 707    | LDA  | C3-C4-C5-C6     |
| 6   | M     | 714    | LDA  | C4-C5-C6-C7     |
| 9   | C     | 355    | HTO  | C1-C2-C3-O3     |
| 9   | C     | 357    | HTO  | C1-C2-C3-O3     |
| 9   | L     | 279    | HTO  | C1-C2-C3-O3     |
| 11  | L     | 401    | BCB  | C2C-C3C-CAC-CBC |
| 13  | L     | 502    | UQ9  | C18-C19-C21-C22 |
| 5   | C     | 402    | HEC  | CAD-CBD-CGD-O2D |
| 6   | M     | 715    | LDA  | C3-C4-C5-C6     |
| 7   | C     | 730    | DGA  | CB9-CAB-CBB-CCB |
| 10  | H     | 281    | GOL  | O1-C1-C2-C3     |
| 5   | C     | 404    | HEC  | CAD-CBD-CGD-O1D |
| 9   | M     | 333    | HTO  | C2-C3-C4-C5     |
| 13  | L     | 502    | UQ9  | C35-C34-C36-C37 |
| 6   | M     | 713    | LDA  | C9-C10-C11-C12  |
| 11  | M     | 401    | BCB  | C14-C13-C15-C16 |
| 6   | H     | 721    | LDA  | C2-C1-N1-O1     |
| 13  | L     | 502    | UQ9  | C38-C39-C41-C42 |
| 11  | L     | 401    | BCB  | CAD-CBD-CGD-O2D |
| 6   | H     | 721    | LDA  | C1-C2-C3-C4     |
| 6   | H     | 719    | LDA  | C7-C8-C9-C10    |
| 5   | C     | 401    | HEC  | CAD-CBD-CGD-O2D |

There are no ring outliers.

45 monomers are involved in 99 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6   | L     | 712 | LDA  | 1       | 0            |
| 9   | H     | 273 | HTO  | 2       | 0            |
| 10  | H     | 279 | GOL  | 1       | 0            |
| 10  | C     | 368 | GOL  | 1       | 0            |
| 6   | L     | 710 | LDA  | 1       | 0            |
| 6   | L     | 724 | LDA  | 2       | 0            |

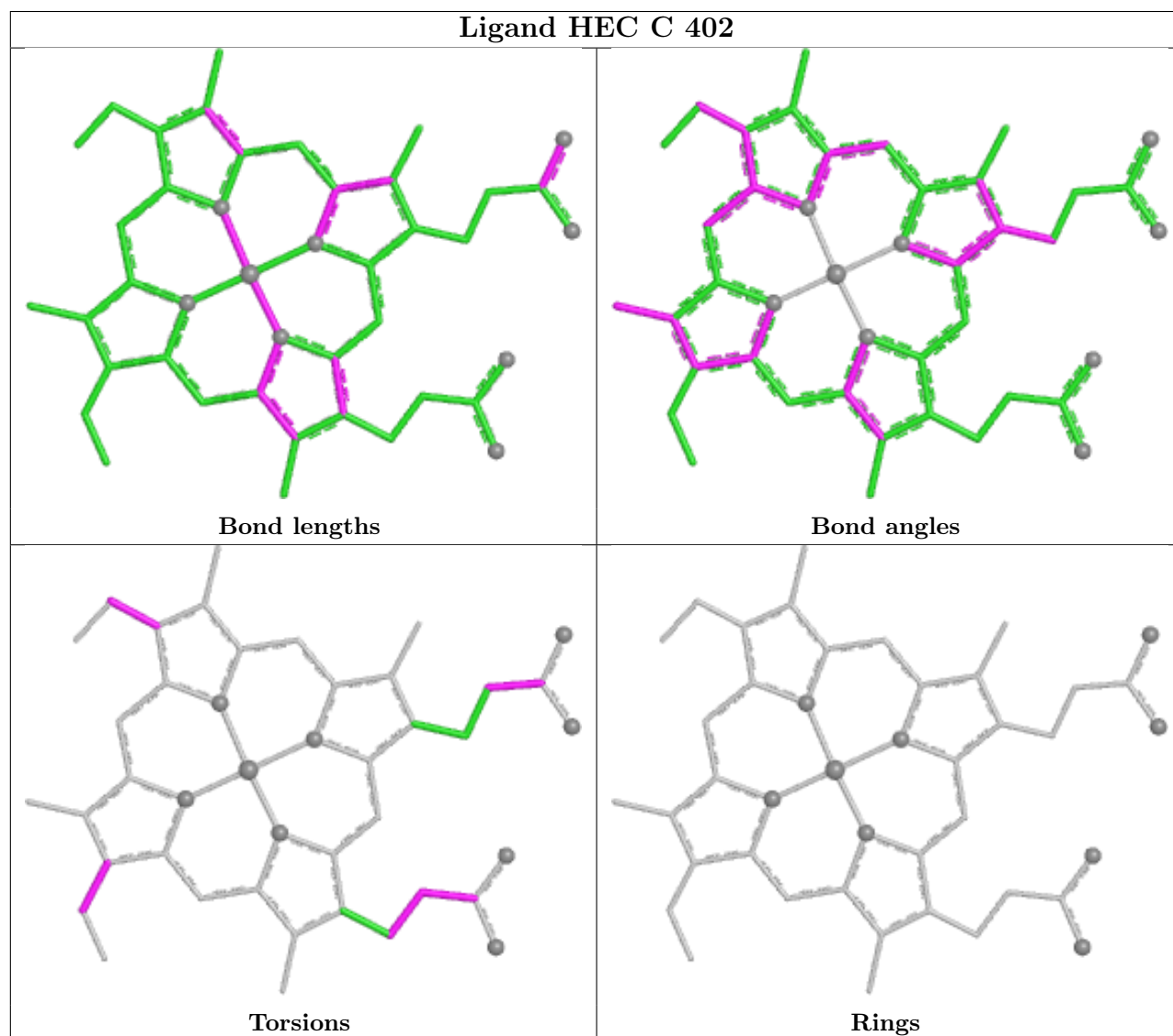
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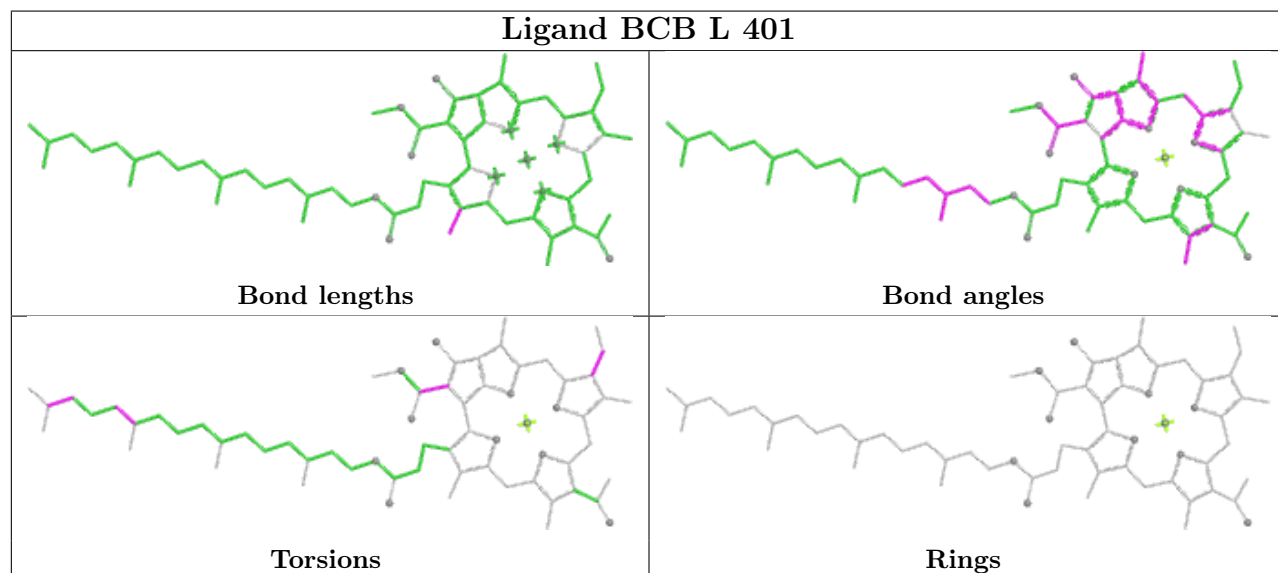
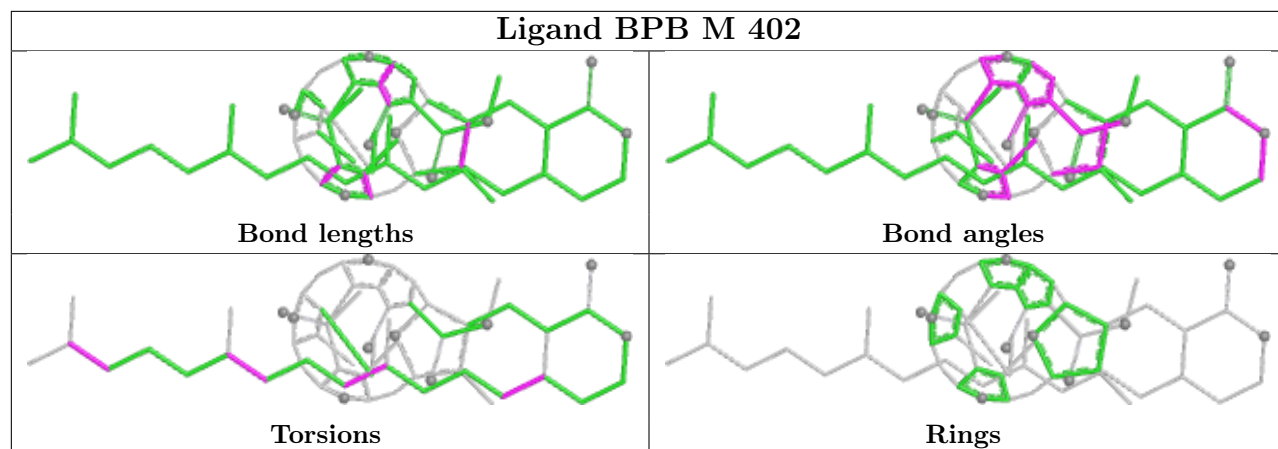
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| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 11  | L     | 401    | BCB  | 4       | 0            |
| 5   | C     | 401    | HEC  | 1       | 0            |
| 11  | M     | 400    | BCB  | 13      | 0            |
| 10  | C     | 363    | GOL  | 1       | 0            |
| 10  | H     | 280    | GOL  | 1       | 0            |
| 10  | C     | 364    | GOL  | 3       | 0            |
| 10  | C     | 365    | GOL  | 2       | 0            |
| 8   | C     | 338    | SO4  | 1       | 0            |
| 10  | L     | 286    | GOL  | 1       | 0            |
| 9   | C     | 357    | HTO  | 2       | 0            |
| 13  | L     | 503    | UQ9  | 5       | 0            |
| 6   | L     | 723    | LDA  | 2       | 0            |
| 7   | C     | 730    | DGA  | 3       | 0            |
| 10  | C     | 377    | GOL  | 4       | 0            |
| 10  | M     | 338    | GOL  | 3       | 0            |
| 10  | M     | 334    | GOL  | 1       | 0            |
| 10  | C     | 373    | GOL  | 1       | 0            |
| 9   | H     | 272    | HTO  | 1       | 0            |
| 6   | M     | 704    | LDA  | 6       | 0            |
| 6   | M     | 714    | LDA  | 2       | 0            |
| 9   | L     | 277    | HTO  | 2       | 0            |
| 6   | L     | 702    | LDA  | 1       | 0            |
| 6   | M     | 715    | LDA  | 2       | 0            |
| 10  | C     | 369    | GOL  | 1       | 0            |
| 11  | L     | 400    | BCB  | 5       | 0            |
| 15  | M     | 501    | MQ9  | 2       | 0            |
| 16  | M     | 600    | NS5  | 3       | 0            |
| 8   | M     | 326    | SO4  | 2       | 0            |
| 10  | H     | 278    | GOL  | 2       | 0            |
| 13  | L     | 502    | UQ9  | 11      | 0            |
| 11  | M     | 401    | BCB  | 4       | 0            |
| 6   | C     | 716    | LDA  | 3       | 0            |
| 6   | M     | 707    | LDA  | 1       | 0            |
| 9   | L     | 279    | HTO  | 1       | 0            |
| 6   | L     | 711    | LDA  | 1       | 0            |
| 9   | H     | 274[A] | HTO  | 1       | 0            |
| 6   | H     | 721    | LDA  | 1       | 0            |
| 10  | M     | 342    | GOL  | 1       | 0            |
| 9   | C     | 355    | HTO  | 6       | 0            |

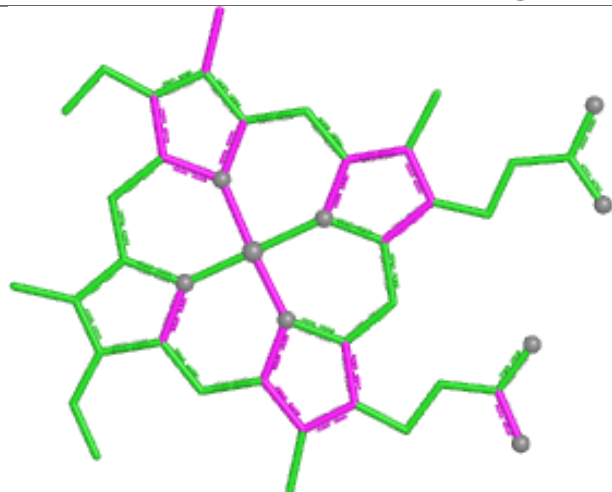
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

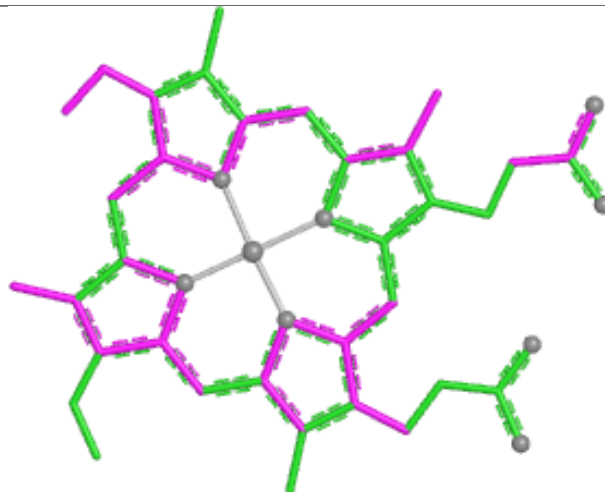




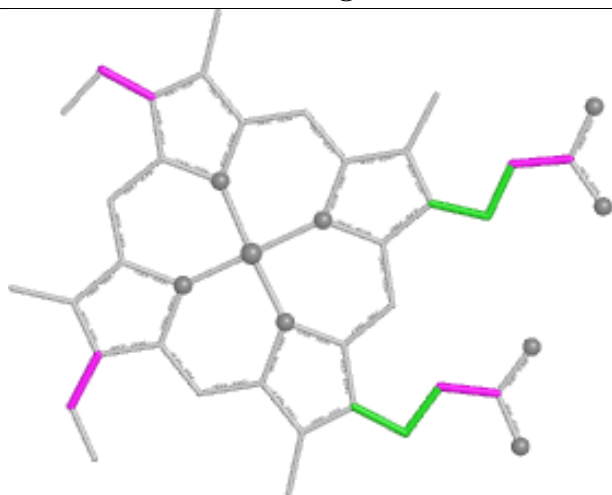
## Ligand HEC C 401



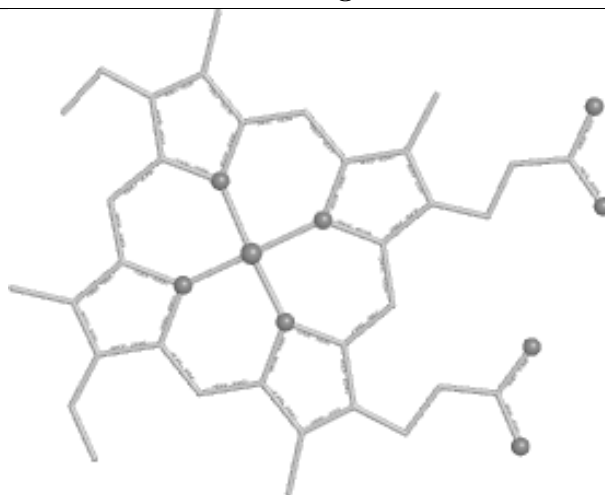
Bond lengths



Bond angles

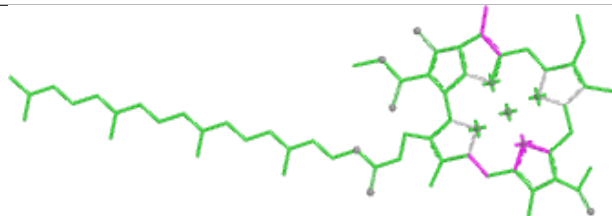


Torsions

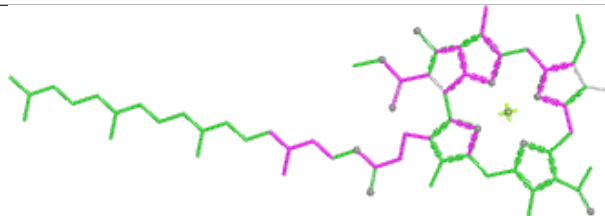


Rings

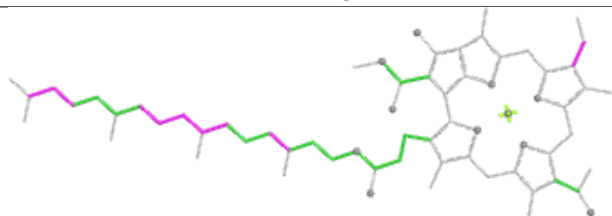
## Ligand BCB M 400



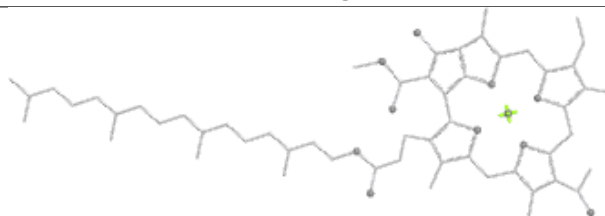
Bond lengths



Bond angles

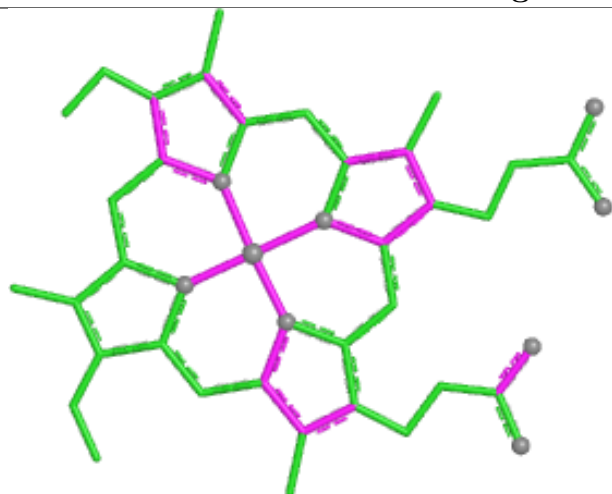


Torsions

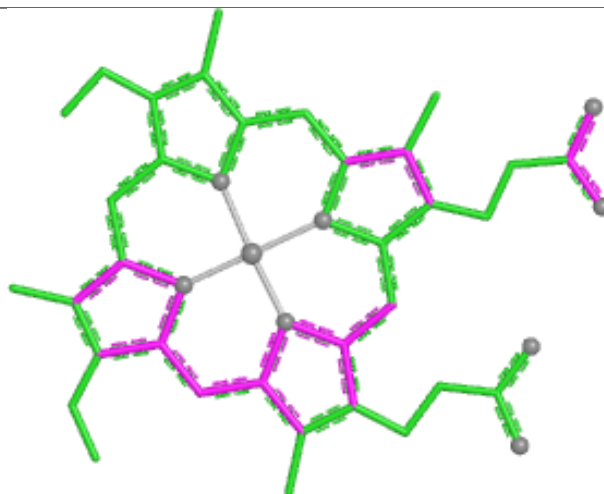


Rings

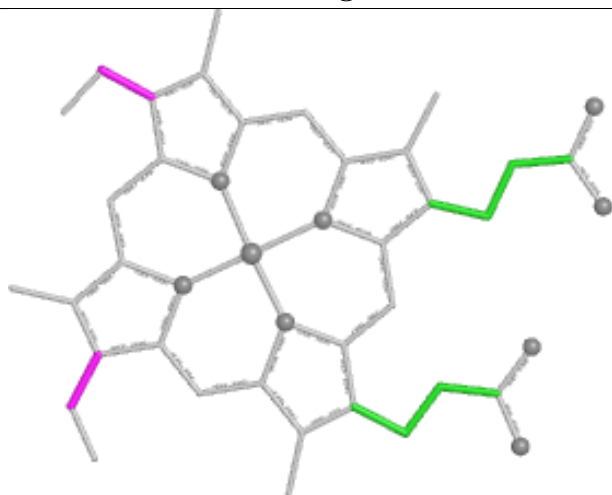
## Ligand HEC C 403



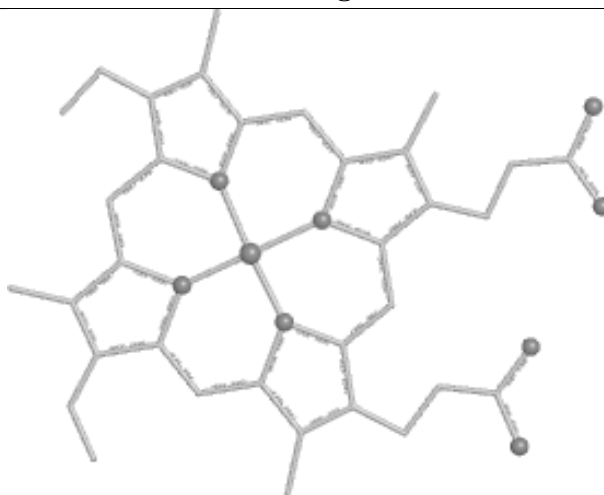
Bond lengths



Bond angles

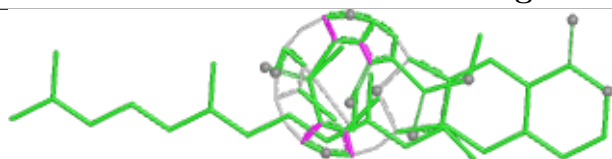


Torsions

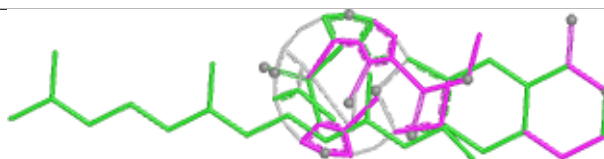


Rings

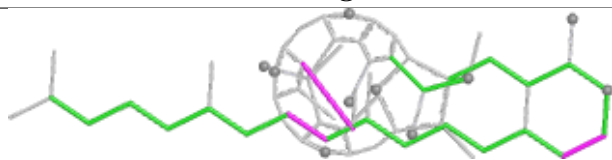
## Ligand BPB L 402



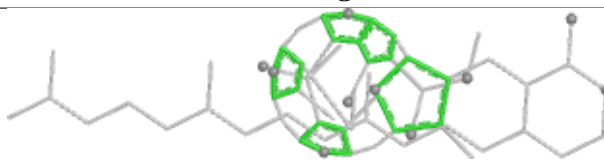
Bond lengths



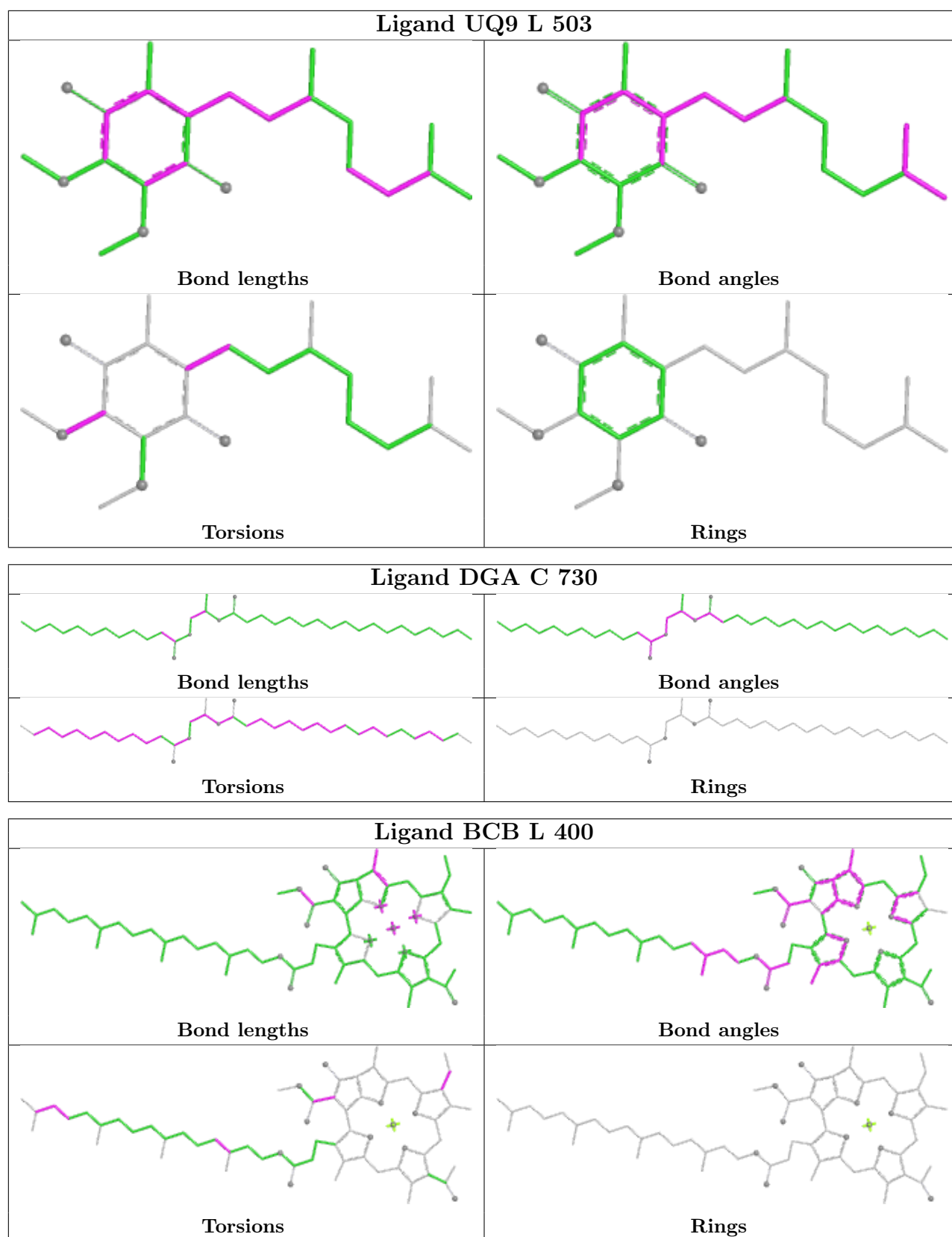
Bond angles

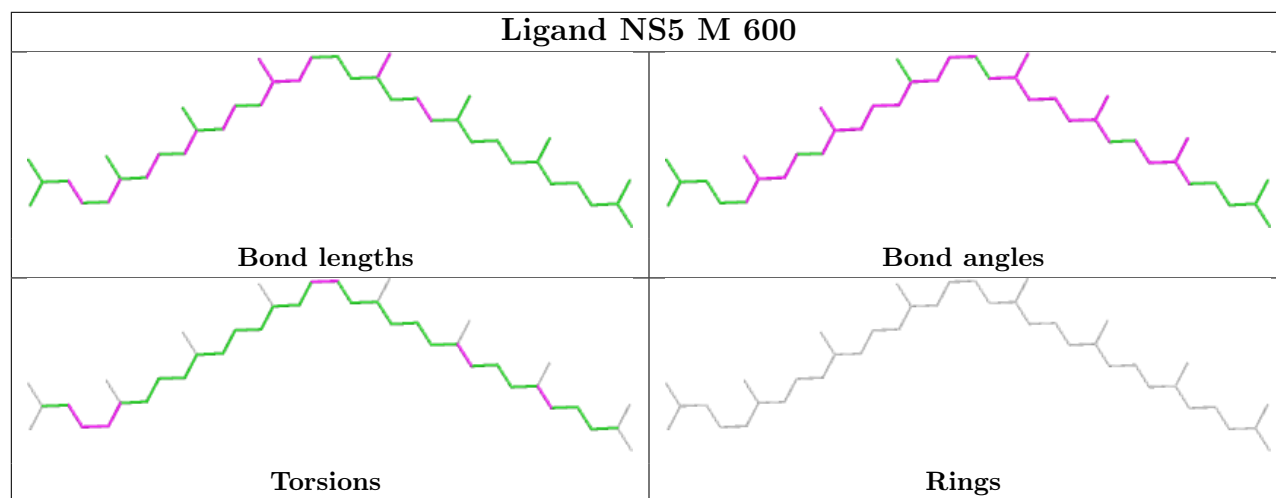
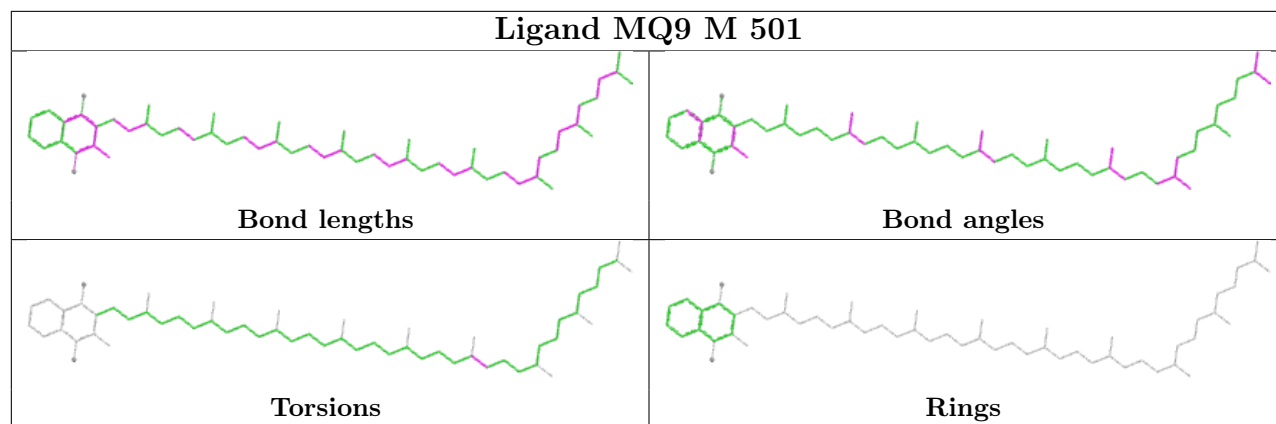


Torsions

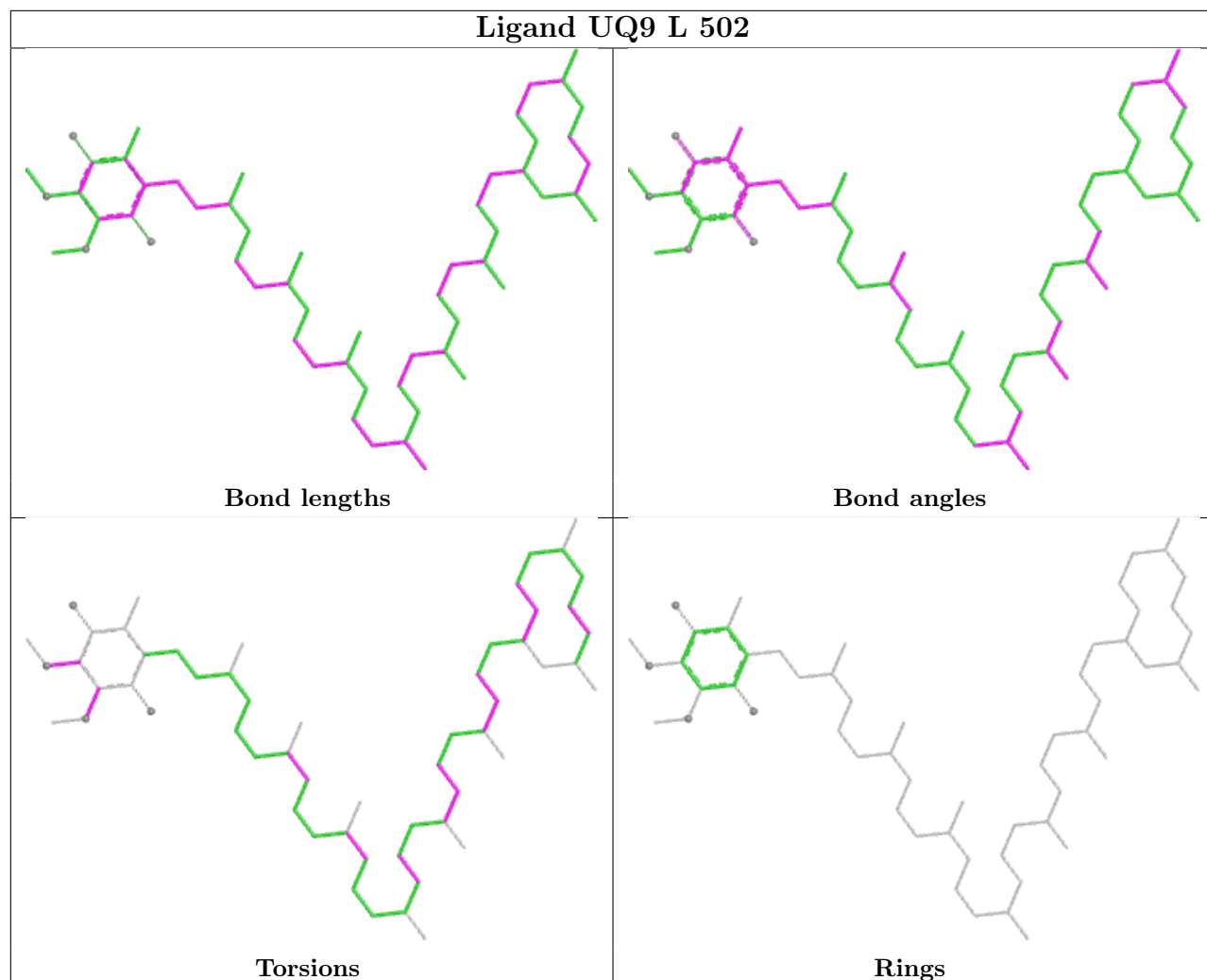


Rings

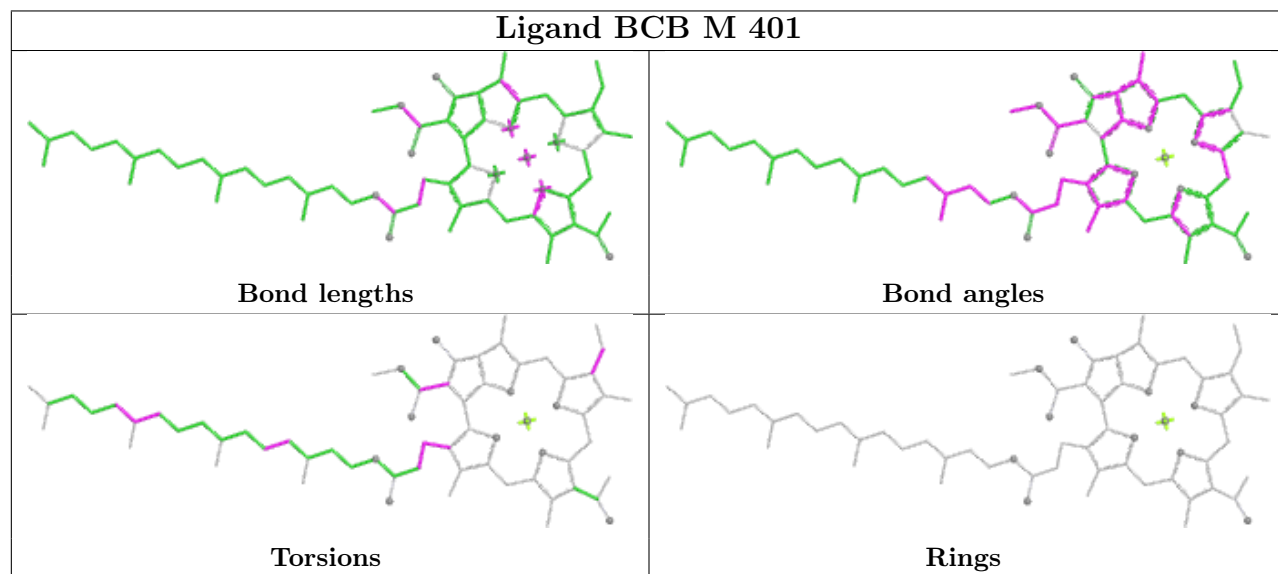


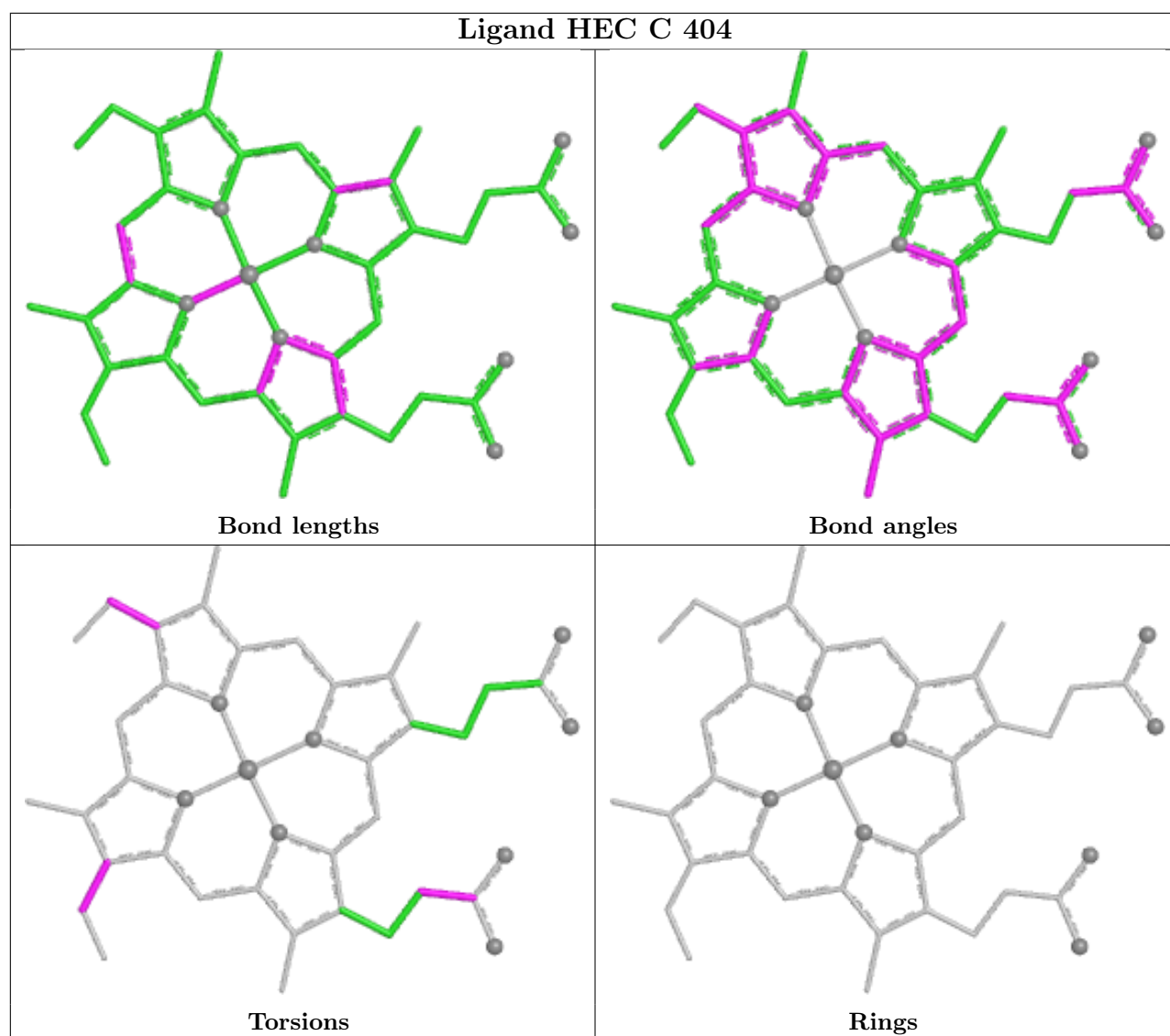


## Ligand UQ9 L 502



## Ligand BCB M 401





## 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   | C     | 334/356 (93%)   | 0.34   | 8 (2%) 59 66  | 26, 45, 68, 125       | 3 (0%)  |
| 2   | H     | 249/258 (96%)   | 0.56   | 16 (6%) 25 29 | 27, 50, 80, 119       | 3 (1%)  |
| 3   | L     | 273/273 (100%)  | 0.28   | 8 (2%) 53 60  | 21, 42, 58, 82        | 2 (0%)  |
| 4   | M     | 323/323 (100%)  | 0.40   | 19 (5%) 28 32 | 26, 43, 65, 83        | 2 (0%)  |
| All | All   | 1179/1210 (97%) | 0.39   | 51 (4%) 40 46 | 21, 45, 69, 125       | 10 (0%) |

All (51) RSRZ outliers are listed below:

| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | C     | 334   | ALA  | 4.4  |
| 3   | L     | 273   | SER  | 4.4  |
| 1   | C     | 1     | CYS  | 4.3  |
| 1   | C     | 333   | ALA  | 4.2  |
| 2   | H     | 85    | THR  | 3.9  |
| 4   | M     | 85[A] | PHE  | 3.8  |
| 4   | M     | 34    | TYR  | 3.7  |
| 1   | C     | 2[A]  | PHE  | 3.6  |
| 3   | L     | 271   | PHE  | 3.6  |
| 3   | L     | 1     | ALA  | 3.6  |
| 2   | H     | 86    | ARG  | 3.4  |
| 4   | M     | 1     | ALA  | 3.4  |
| 3   | L     | 202   | ASP  | 3.3  |
| 2   | H     | 96    | PHE  | 3.3  |
| 2   | H     | 44    | VAL  | 3.2  |
| 2   | H     | 189   | GLY  | 3.2  |
| 4   | M     | 37    | TRP  | 3.2  |
| 2   | H     | 45    | GLU  | 3.2  |
| 4   | M     | 108   | HIS  | 3.1  |
| 2   | H     | 54    | PRO  | 3.1  |
| 3   | L     | 81    | LEU  | 3.0  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 2   | H     | 177    | GLU  | 3.0  |
| 3   | L     | 270    | PRO  | 2.9  |
| 4   | M     | 26     | ASN  | 2.9  |
| 3   | L     | 51[A]  | TYR  | 2.8  |
| 1   | C     | 47     | ALA  | 2.8  |
| 4   | M     | 33     | PHE  | 2.8  |
| 4   | M     | 16     | HIS  | 2.7  |
| 2   | H     | 178[A] | HIS  | 2.7  |
| 2   | H     | 43     | LEU  | 2.6  |
| 3   | L     | 21     | LEU  | 2.6  |
| 2   | H     | 64     | TYR  | 2.5  |
| 4   | M     | 118    | LEU  | 2.5  |
| 4   | M     | 18     | THR  | 2.5  |
| 1   | C     | 89     | TYR  | 2.5  |
| 4   | M     | 31     | LYS  | 2.4  |
| 2   | H     | 190    | SER  | 2.4  |
| 1   | C     | 323    | GLN  | 2.3  |
| 1   | C     | 55     | VAL  | 2.3  |
| 4   | M     | 20     | SER  | 2.3  |
| 2   | H     | 8      | GLN  | 2.3  |
| 4   | M     | 115    | MET  | 2.3  |
| 4   | M     | 78     | HIS  | 2.2  |
| 4   | M     | 319    | PRO  | 2.2  |
| 4   | M     | 59     | PHE  | 2.2  |
| 2   | H     | 257    | LEU  | 2.2  |
| 4   | M     | 17     | ILE  | 2.1  |
| 4   | M     | 22     | GLU  | 2.1  |
| 2   | H     | 223[A] | ARG  | 2.1  |
| 4   | M     | 32     | PRO  | 2.0  |
| 2   | H     | 83     | PRO  | 2.0  |

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

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 2   | FME  | H     | 1[A] | 10/11 | 0.94 | 0.11 | 47,50,54,56                | 7     |
| 2   | FME  | H     | 1[B] | 10/11 | 0.94 | 0.11 | 47,53,59,61                | 7     |

## 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|----------------------------|-------|
| 9   | HTO  | H     | 274[A] | 10/10 | 0.58 | 0.43 | 53,69,72,75                | 10    |
| 9   | HTO  | L     | 279    | 10/10 | 0.71 | 0.44 | 65,66,69,75                | 10    |
| 6   | LDA  | H     | 718[B] | 16/16 | 0.72 | 0.56 | 50,80,89,90                | 16    |
| 10  | GOL  | H     | 279    | 6/6   | 0.72 | 0.27 | 63,68,71,72                | 6     |
| 10  | GOL  | M     | 342    | 6/6   | 0.73 | 0.34 | 66,67,69,70                | 6     |
| 10  | GOL  | C     | 372    | 6/6   | 0.74 | 0.35 | 56,62,65,65                | 6     |
| 8   | SO4  | C     | 344    | 5/5   | 0.75 | 0.17 | 74,76,79,82                | 5     |
| 6   | LDA  | L     | 711    | 16/16 | 0.76 | 0.35 | 60,68,76,77                | 16    |
| 8   | SO4  | C     | 342    | 5/5   | 0.76 | 0.15 | 63,68,71,75                | 5     |
| 6   | LDA  | C     | 716    | 16/16 | 0.77 | 0.36 | 50,65,72,74                | 16    |
| 10  | GOL  | C     | 376    | 6/6   | 0.77 | 0.22 | 63,74,77,83                | 6     |
| 17  | HTH  | M     | 332    | 10/10 | 0.77 | 0.40 | 58,68,76,77                | 10    |
| 10  | GOL  | H     | 287    | 6/6   | 0.78 | 0.32 | 65,71,72,73                | 6     |
| 9   | HTO  | L     | 280    | 10/10 | 0.78 | 0.38 | 63,69,71,72                | 10    |
| 9   | HTO  | C     | 355    | 10/10 | 0.78 | 0.27 | 62,66,71,72                | 10    |
| 10  | GOL  | H     | 280    | 6/6   | 0.79 | 0.27 | 52,60,65,66                | 6     |
| 6   | LDA  | M     | 706    | 16/16 | 0.80 | 0.42 | 49,55,65,68                | 16    |
| 8   | SO4  | C     | 348    | 5/5   | 0.80 | 0.25 | 70,73,77,80                | 5     |
| 8   | SO4  | M     | 331    | 5/5   | 0.80 | 0.16 | 60,60,61,62                | 5     |
| 10  | GOL  | H     | 283    | 6/6   | 0.80 | 0.34 | 59,60,61,61                | 6     |
| 10  | GOL  | C     | 370    | 6/6   | 0.80 | 0.42 | 64,66,68,68                | 6     |
| 10  | GOL  | L     | 286    | 6/6   | 0.80 | 0.30 | 58,63,64,68                | 6     |
| 6   | LDA  | L     | 712    | 16/16 | 0.80 | 0.40 | 51,64,70,71                | 16    |
| 13  | UQ9  | L     | 503    | 23/58 | 0.80 | 0.30 | 59,73,85,87                | 23    |
| 10  | GOL  | C     | 373    | 6/6   | 0.80 | 0.41 | 60,63,64,65                | 6     |
| 9   | HTO  | L     | 278    | 10/10 | 0.81 | 0.30 | 57,65,67,69                | 10    |
| 6   | LDA  | L     | 702    | 16/16 | 0.81 | 0.34 | 51,53,57,57                | 16    |
| 10  | GOL  | L     | 288    | 6/6   | 0.81 | 0.49 | 54,57,58,60                | 6     |
| 10  | GOL  | M     | 341    | 6/6   | 0.81 | 0.43 | 68,71,74,75                | 6     |
| 6   | LDA  | M     | 717    | 16/16 | 0.81 | 0.35 | 50,59,89,91                | 16    |
| 10  | GOL  | C     | 374[B] | 6/6   | 0.81 | 0.42 | 66,67,68,68                | 6     |
| 10  | GOL  | H     | 285    | 6/6   | 0.81 | 0.36 | 68,70,71,71                | 6     |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 7   | DGA  | C     | 730    | 37/44 | 0.82 | 0.28 | 112,125,144,151             | 0     |
| 8   | SO4  | H     | 270    | 5/5   | 0.82 | 0.35 | 60,61,63,63                 | 5     |
| 10  | GOL  | H     | 288    | 6/6   | 0.82 | 0.39 | 60,68,68,73                 | 6     |
| 10  | GOL  | H     | 291    | 6/6   | 0.82 | 0.19 | 74,78,80,81                 | 6     |
| 9   | HTO  | C     | 357    | 10/10 | 0.82 | 0.36 | 59,65,73,80                 | 10    |
| 9   | HTO  | C     | 358[A] | 10/10 | 0.82 | 0.43 | 58,62,67,68                 | 10    |
| 10  | GOL  | C     | 363    | 6/6   | 0.82 | 0.26 | 46,59,65,69                 | 6     |
| 10  | GOL  | C     | 368    | 6/6   | 0.82 | 0.30 | 62,63,68,70                 | 6     |
| 10  | GOL  | H     | 281    | 6/6   | 0.82 | 0.28 | 64,67,72,76                 | 6     |
| 9   | HTO  | H     | 272    | 10/10 | 0.82 | 0.23 | 61,67,75,80                 | 10    |
| 10  | GOL  | C     | 371    | 6/6   | 0.83 | 0.39 | 55,62,62,63                 | 6     |
| 8   | SO4  | H     | 271    | 5/5   | 0.83 | 0.34 | 64,64,65,68                 | 5     |
| 8   | SO4  | C     | 340    | 5/5   | 0.83 | 0.19 | 57,71,76,82                 | 5     |
| 10  | GOL  | C     | 360    | 6/6   | 0.83 | 0.19 | 44,56,62,71                 | 6     |
| 10  | GOL  | C     | 375    | 6/6   | 0.83 | 0.42 | 66,69,70,72                 | 6     |
| 10  | GOL  | L     | 285    | 6/6   | 0.84 | 0.27 | 51,67,70,71                 | 6     |
| 6   | LDA  | C     | 722    | 16/16 | 0.84 | 0.31 | 53,63,66,66                 | 16    |
| 8   | SO4  | C     | 343    | 5/5   | 0.84 | 0.18 | 52,62,65,66                 | 5     |
| 8   | SO4  | M     | 327    | 5/5   | 0.84 | 0.15 | 53,58,68,75                 | 5     |
| 8   | SO4  | C     | 339    | 5/5   | 0.84 | 0.15 | 69,71,75,80                 | 5     |
| 8   | SO4  | C     | 347    | 5/5   | 0.84 | 0.20 | 78,82,83,90                 | 5     |
| 6   | LDA  | L     | 710    | 16/16 | 0.84 | 0.32 | 52,60,81,82                 | 16    |
| 8   | SO4  | C     | 346    | 5/5   | 0.85 | 0.26 | 57,65,71,72                 | 5     |
| 10  | GOL  | M     | 336    | 6/6   | 0.85 | 0.34 | 68,69,70,71                 | 6     |
| 10  | GOL  | M     | 340    | 6/6   | 0.85 | 0.26 | 60,64,65,66                 | 6     |
| 10  | GOL  | H     | 277    | 6/6   | 0.85 | 0.23 | 55,59,62,62                 | 6     |
| 10  | GOL  | L     | 282    | 6/6   | 0.85 | 0.24 | 53,59,59,63                 | 6     |
| 6   | LDA  | M     | 704    | 16/16 | 0.85 | 0.31 | 49,80,87,87                 | 16    |
| 8   | SO4  | M     | 330    | 5/5   | 0.85 | 0.20 | 67,68,68,69                 | 5     |
| 10  | GOL  | C     | 364    | 6/6   | 0.86 | 0.22 | 52,67,67,68                 | 6     |
| 10  | GOL  | H     | 276[A] | 6/6   | 0.86 | 0.17 | 50,60,62,62                 | 2     |
| 10  | GOL  | L     | 284    | 6/6   | 0.86 | 0.21 | 52,65,67,67                 | 6     |
| 10  | GOL  | H     | 276[B] | 6/6   | 0.86 | 0.17 | 50,59,60,62                 | 2     |
| 10  | GOL  | C     | 366    | 6/6   | 0.86 | 0.28 | 56,62,63,71                 | 6     |
| 10  | GOL  | L     | 287    | 6/6   | 0.86 | 0.23 | 54,55,57,57                 | 6     |
| 6   | LDA  | L     | 723    | 16/16 | 0.86 | 0.44 | 55,58,64,68                 | 16    |
| 6   | LDA  | M     | 715    | 16/16 | 0.86 | 0.33 | 58,71,77,79                 | 16    |
| 10  | GOL  | M     | 338    | 6/6   | 0.86 | 0.33 | 57,60,62,63                 | 6     |
| 9   | HTO  | C     | 356    | 10/10 | 0.86 | 0.30 | 59,72,76,77                 | 10    |
| 6   | LDA  | H     | 720    | 16/16 | 0.86 | 0.27 | 55,69,73,73                 | 16    |
| 8   | SO4  | M     | 328    | 5/5   | 0.86 | 0.23 | 61,62,64,69                 | 5     |
| 10  | GOL  | C     | 361    | 6/6   | 0.86 | 0.26 | 60,64,72,75                 | 6     |

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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 8   | SO4  | C     | 349    | 5/5   | 0.86 | 0.20 | 63,64,71,71                 | 5     |
| 10  | GOL  | L     | 283    | 6/6   | 0.87 | 0.20 | 59,63,68,70                 | 6     |
| 8   | SO4  | C     | 350    | 5/5   | 0.87 | 0.25 | 64,67,69,72                 | 5     |
| 10  | GOL  | C     | 367    | 6/6   | 0.87 | 0.34 | 50,58,59,60                 | 6     |
| 8   | SO4  | C     | 353    | 5/5   | 0.87 | 0.18 | 66,69,72,76                 | 5     |
| 8   | SO4  | H     | 263    | 5/5   | 0.87 | 0.20 | 75,76,78,79                 | 5     |
| 8   | SO4  | H     | 265    | 5/5   | 0.87 | 0.15 | 69,74,75,81                 | 5     |
| 9   | HTO  | M     | 333    | 10/10 | 0.87 | 0.30 | 44,51,55,55                 | 10    |
| 10  | GOL  | H     | 284    | 6/6   | 0.87 | 0.34 | 58,63,65,68                 | 6     |
| 10  | GOL  | M     | 339    | 6/6   | 0.87 | 0.32 | 60,65,66,66                 | 6     |
| 8   | SO4  | H     | 268    | 5/5   | 0.87 | 0.39 | 63,66,70,72                 | 5     |
| 6   | LDA  | M     | 714    | 16/16 | 0.87 | 0.35 | 70,75,81,82                 | 16    |
| 8   | SO4  | C     | 337[A] | 5/5   | 0.87 | 0.21 | 59,62,67,67                 | 5     |
| 13  | UQ9  | L     | 502    | 58/58 | 0.87 | 0.25 | 44,80,97,99                 | 58    |
| 8   | SO4  | C     | 337[B] | 5/5   | 0.87 | 0.21 | 59,64,69,70                 | 5     |
| 10  | GOL  | C     | 365    | 6/6   | 0.87 | 0.17 | 60,67,69,72                 | 6     |
| 6   | LDA  | H     | 719    | 16/16 | 0.88 | 0.27 | 58,63,71,72                 | 16    |
| 10  | GOL  | C     | 377    | 6/6   | 0.88 | 0.20 | 63,65,67,67                 | 6     |
| 10  | GOL  | C     | 369    | 6/6   | 0.88 | 0.29 | 49,56,61,61                 | 6     |
| 9   | HTO  | H     | 273    | 10/10 | 0.88 | 0.32 | 48,51,60,62                 | 10    |
| 10  | GOL  | H     | 289    | 6/6   | 0.88 | 0.31 | 62,66,66,67                 | 6     |
| 6   | LDA  | L     | 724    | 16/16 | 0.88 | 0.33 | 53,63,68,69                 | 16    |
| 10  | GOL  | H     | 278    | 6/6   | 0.88 | 0.17 | 63,67,68,71                 | 6     |
| 8   | SO4  | C     | 345    | 5/5   | 0.88 | 0.13 | 66,68,72,72                 | 5     |
| 8   | SO4  | C     | 341    | 5/5   | 0.88 | 0.12 | 67,74,80,81                 | 5     |
| 8   | SO4  | C     | 338    | 5/5   | 0.88 | 0.13 | 53,57,60,64                 | 5     |
| 8   | SO4  | H     | 264    | 5/5   | 0.88 | 0.25 | 61,67,72,73                 | 5     |
| 6   | LDA  | L     | 703    | 16/16 | 0.89 | 0.25 | 52,57,61,63                 | 16    |
| 6   | LDA  | M     | 707    | 16/16 | 0.89 | 0.26 | 42,58,72,81                 | 16    |
| 8   | SO4  | H     | 269    | 5/5   | 0.89 | 0.25 | 71,72,75,76                 | 5     |
| 9   | HTO  | L     | 276    | 10/10 | 0.89 | 0.25 | 50,67,70,71                 | 10    |
| 8   | SO4  | M     | 329    | 5/5   | 0.89 | 0.25 | 57,58,63,67                 | 5     |
| 10  | GOL  | M     | 337    | 6/6   | 0.89 | 0.30 | 68,69,69,70                 | 6     |
| 6   | LDA  | M     | 705    | 16/16 | 0.89 | 0.25 | 61,69,87,87                 | 16    |
| 8   | SO4  | C     | 354    | 5/5   | 0.90 | 0.29 | 66,69,70,71                 | 5     |
| 10  | GOL  | H     | 282    | 6/6   | 0.90 | 0.26 | 59,66,68,69                 | 6     |
| 6   | LDA  | L     | 709    | 16/16 | 0.90 | 0.23 | 39,63,93,97                 | 16    |
| 10  | GOL  | C     | 378    | 6/6   | 0.90 | 0.27 | 78,80,81,81                 | 6     |
| 10  | GOL  | M     | 334    | 6/6   | 0.90 | 0.17 | 40,56,66,69                 | 6     |
| 10  | GOL  | H     | 290    | 6/6   | 0.91 | 0.26 | 49,59,63,67                 | 6     |
| 8   | SO4  | H     | 260    | 5/5   | 0.91 | 0.09 | 59,63,68,71                 | 5     |
| 10  | GOL  | C     | 362    | 6/6   | 0.91 | 0.19 | 51,57,63,63                 | 6     |

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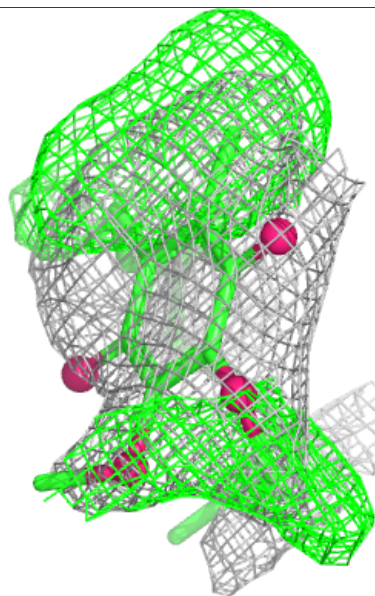
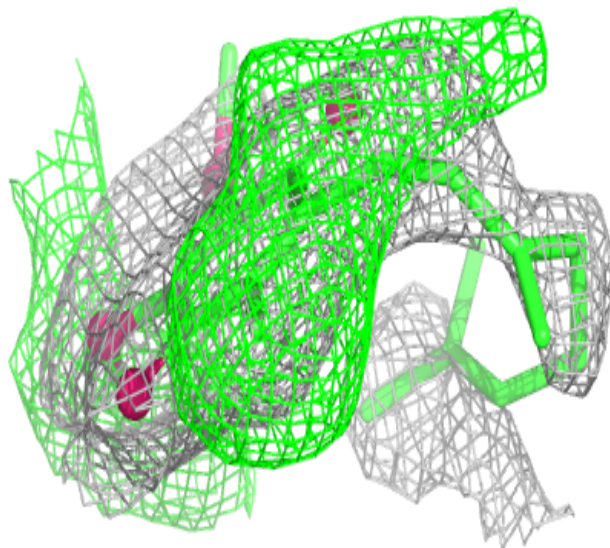
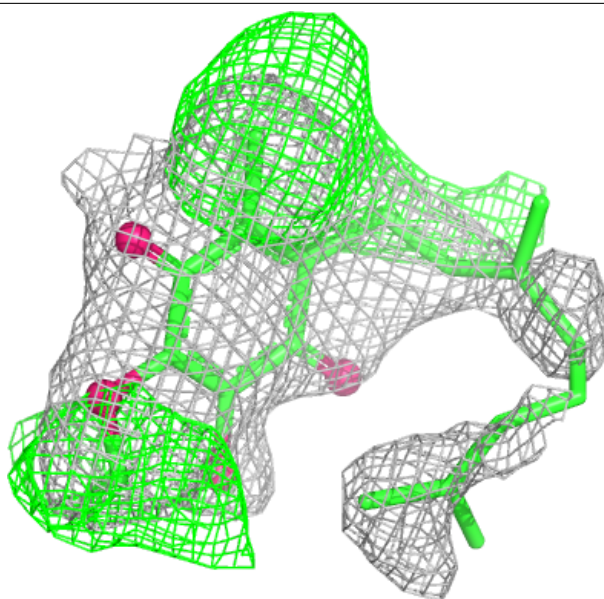
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| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 8   | SO4  | H     | 259    | 5/5   | 0.91 | 0.10 | 60,62,67,69                 | 5     |
| 16  | NS5  | M     | 600    | 40/40 | 0.91 | 0.16 | 42,54,95,96                 | 0     |
| 8   | SO4  | M     | 326    | 5/5   | 0.91 | 0.13 | 56,61,62,62                 | 5     |
| 10  | GOL  | L     | 281    | 6/6   | 0.92 | 0.20 | 54,58,66,68                 | 6     |
| 10  | GOL  | H     | 286    | 6/6   | 0.92 | 0.25 | 67,67,69,70                 | 6     |
| 8   | SO4  | C     | 352    | 5/5   | 0.92 | 0.15 | 78,78,81,82                 | 5     |
| 8   | SO4  | H     | 266    | 5/5   | 0.92 | 0.19 | 65,66,68,71                 | 5     |
| 6   | LDA  | L     | 708    | 16/16 | 0.93 | 0.13 | 40,56,68,76                 | 0     |
| 6   | LDA  | M     | 713    | 16/16 | 0.93 | 0.24 | 63,69,84,86                 | 16    |
| 10  | GOL  | H     | 275    | 6/6   | 0.93 | 0.15 | 59,62,64,67                 | 0     |
| 9   | HTO  | L     | 277    | 10/10 | 0.93 | 0.27 | 57,64,69,76                 | 10    |
| 8   | SO4  | L     | 274    | 5/5   | 0.93 | 0.15 | 62,62,65,68                 | 5     |
| 6   | LDA  | H     | 701    | 16/16 | 0.94 | 0.12 | 43,57,71,73                 | 0     |
| 8   | SO4  | H     | 261[A] | 5/5   | 0.94 | 0.14 | 52,58,64,65                 | 5     |
| 8   | SO4  | H     | 261[B] | 5/5   | 0.94 | 0.14 | 47,54,61,61                 | 5     |
| 8   | SO4  | C     | 351    | 5/5   | 0.94 | 0.15 | 60,60,63,67                 | 5     |
| 11  | BCB  | M     | 400    | 66/66 | 0.95 | 0.11 | 34,40,109,121               | 0     |
| 10  | GOL  | M     | 335    | 6/6   | 0.95 | 0.15 | 44,54,60,68                 | 6     |
| 6   | LDA  | H     | 721    | 16/16 | 0.95 | 0.15 | 50,66,69,69                 | 0     |
| 10  | GOL  | C     | 359    | 6/6   | 0.95 | 0.12 | 44,50,54,55                 | 6     |
| 8   | SO4  | L     | 275    | 5/5   | 0.95 | 0.27 | 66,66,67,68                 | 5     |
| 8   | SO4  | M     | 324    | 5/5   | 0.96 | 0.09 | 47,52,61,63                 | 0     |
| 12  | BPB  | M     | 402    | 65/65 | 0.96 | 0.10 | 33,41,124,132               | 0     |
| 11  | BCB  | L     | 400    | 66/66 | 0.97 | 0.07 | 28,36,48,52                 | 0     |
| 8   | SO4  | H     | 267    | 5/5   | 0.97 | 0.17 | 56,64,65,65                 | 5     |
| 15  | MQ9  | M     | 501    | 58/58 | 0.97 | 0.10 | 31,41,92,98                 | 0     |
| 11  | BCB  | M     | 401    | 66/66 | 0.97 | 0.08 | 28,34,58,66                 | 0     |
| 8   | SO4  | M     | 325    | 5/5   | 0.97 | 0.09 | 64,67,78,79                 | 0     |
| 5   | HEC  | C     | 404    | 43/43 | 0.98 | 0.07 | 32,38,51,64                 | 0     |
| 11  | BCB  | L     | 401    | 66/66 | 0.98 | 0.07 | 27,35,64,75                 | 0     |
| 12  | BPB  | L     | 402    | 65/65 | 0.98 | 0.06 | 32,39,48,51                 | 0     |
| 5   | HEC  | C     | 401    | 43/43 | 0.99 | 0.06 | 41,46,55,58                 | 0     |
| 8   | SO4  | H     | 262    | 5/5   | 0.99 | 0.06 | 41,43,45,47                 | 5     |
| 5   | HEC  | C     | 402    | 43/43 | 0.99 | 0.07 | 39,44,52,60                 | 0     |
| 5   | HEC  | C     | 403    | 43/43 | 0.99 | 0.06 | 32,36,41,42                 | 0     |
| 14  | FE2  | M     | 500    | 1/1   | 1.00 | 0.04 | 37,37,37,37                 | 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.

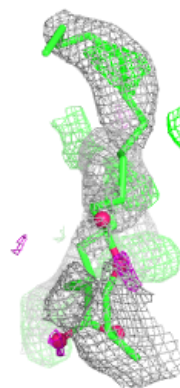
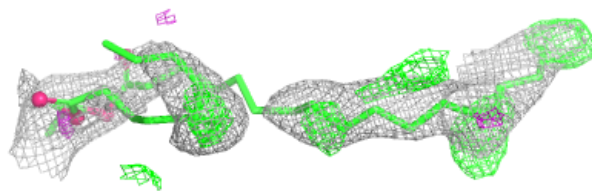
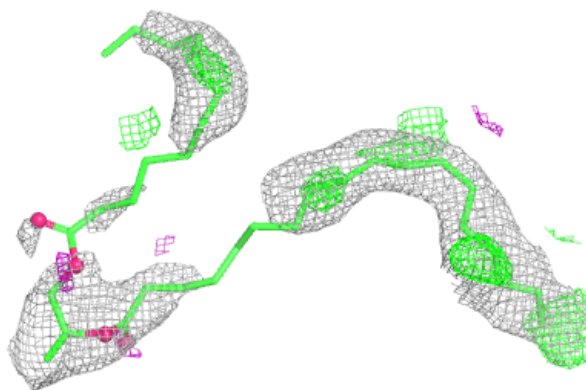
**Electron density around UQ9 L 503:**

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



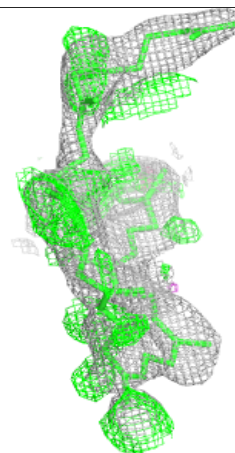
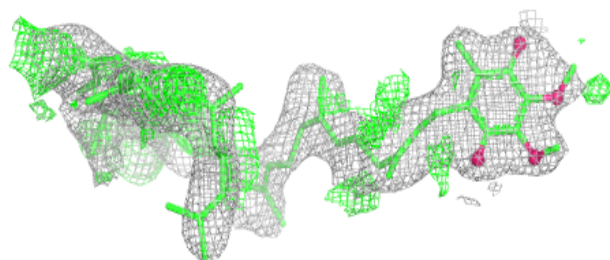
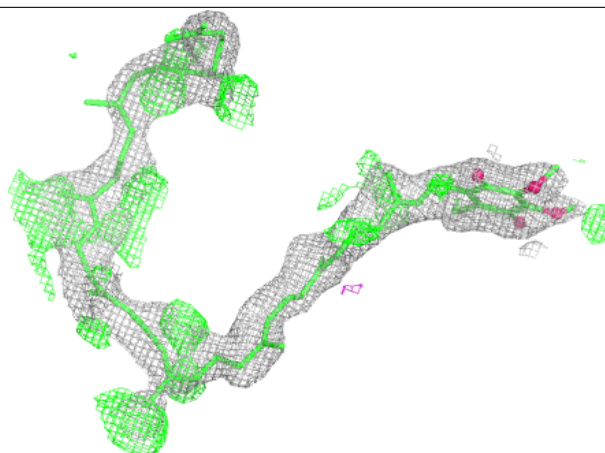
**Electron density around DGA C 730:**

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

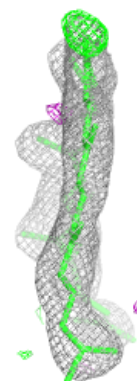
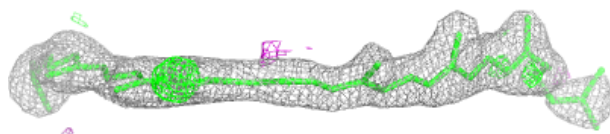
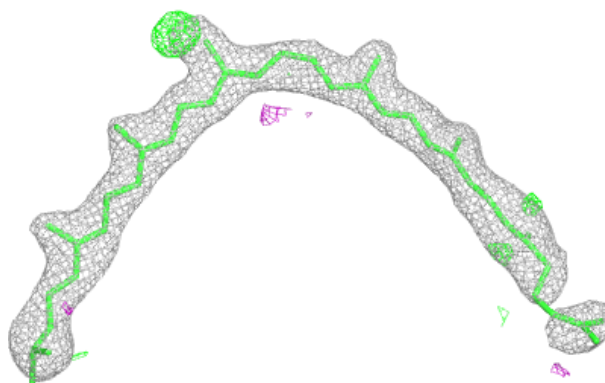


**Electron density around UQ9 L 502:**

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

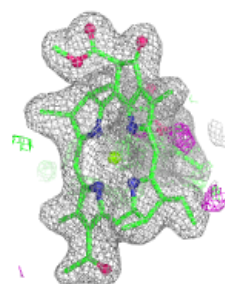
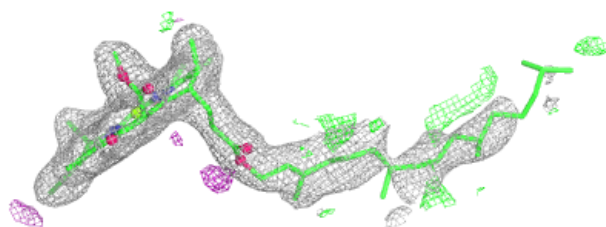
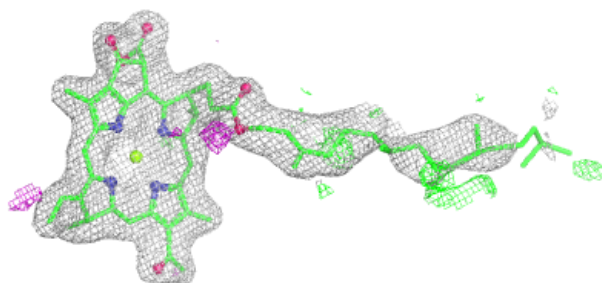
**Electron density around NS5 M 600:**

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

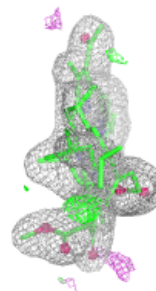
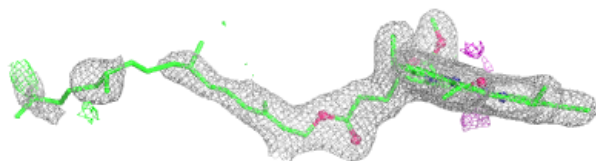
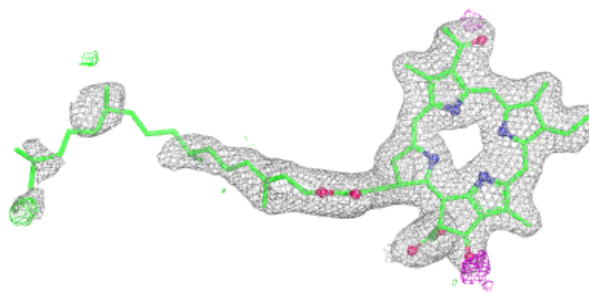


**Electron density around BCB M 400:**

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

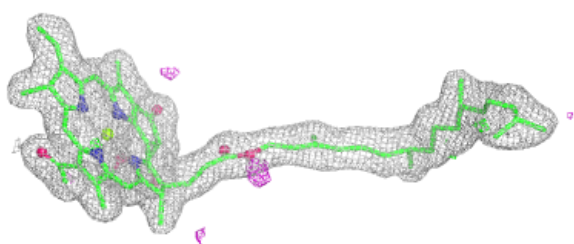
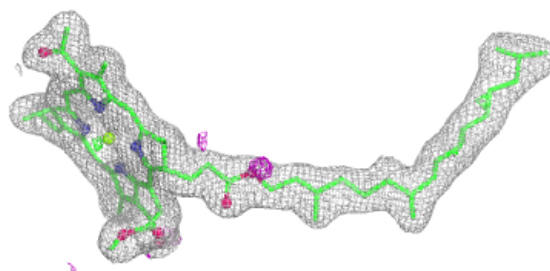
**Electron density around BPB M 402:**

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

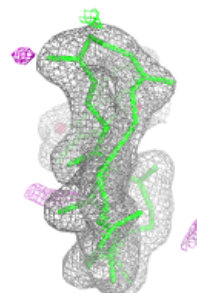
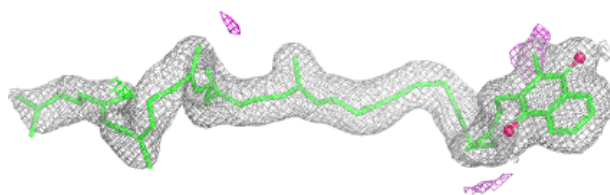
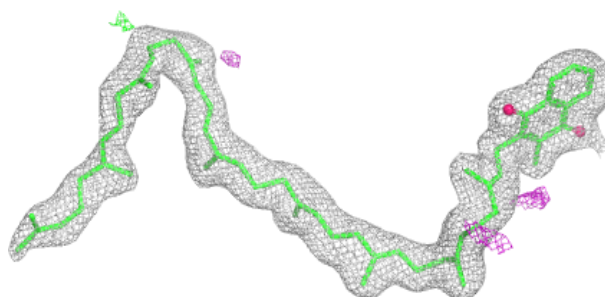


**Electron density around BCB L 400:**

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

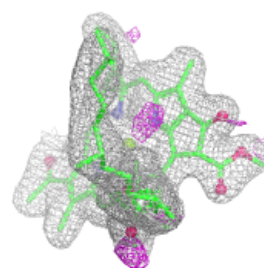
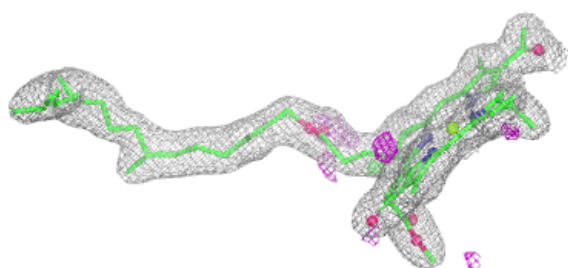
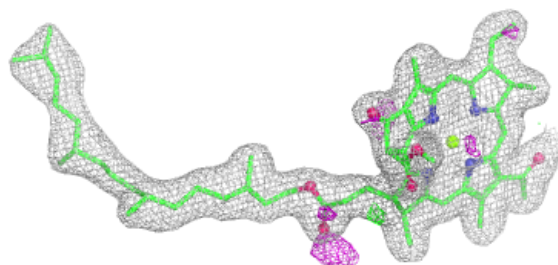
**Electron density around MQ9 M 501:**

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



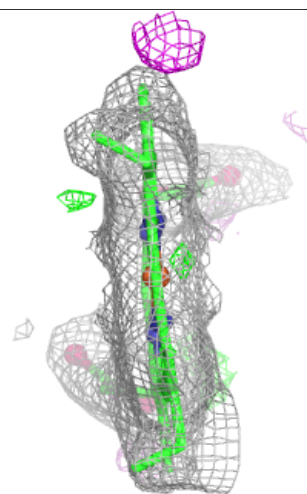
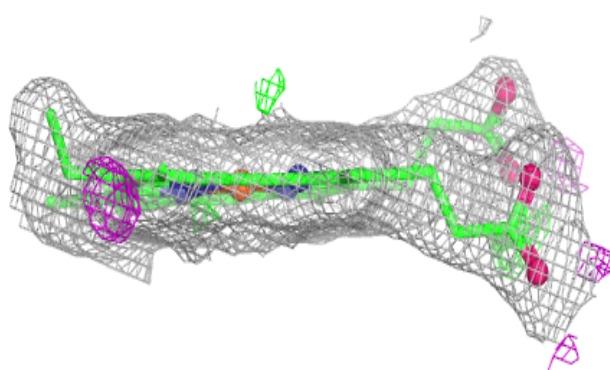
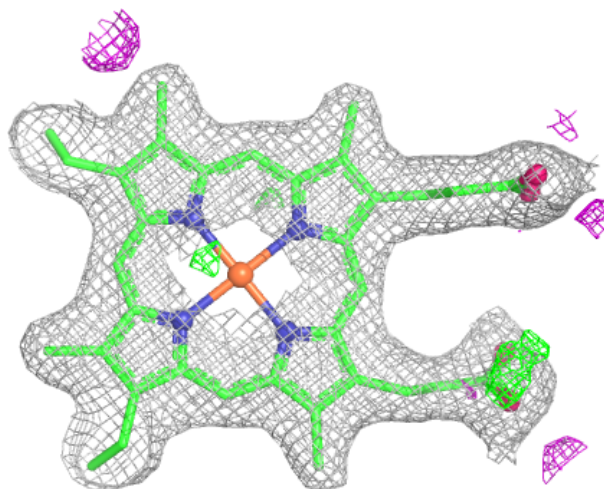
**Electron density around BCB M 401:**

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



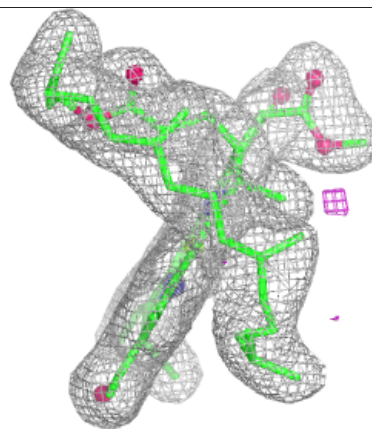
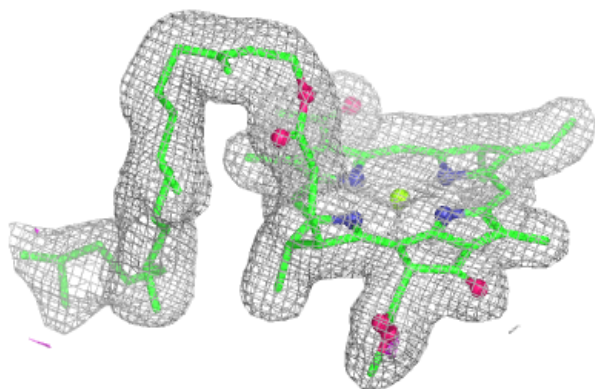
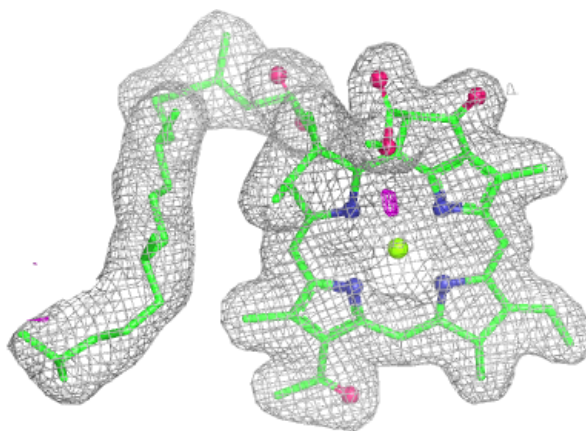
**Electron density around HEC C 404:**

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



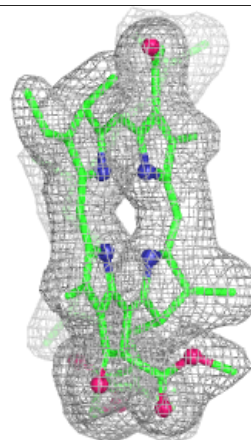
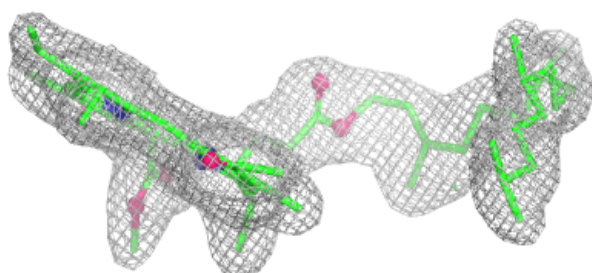
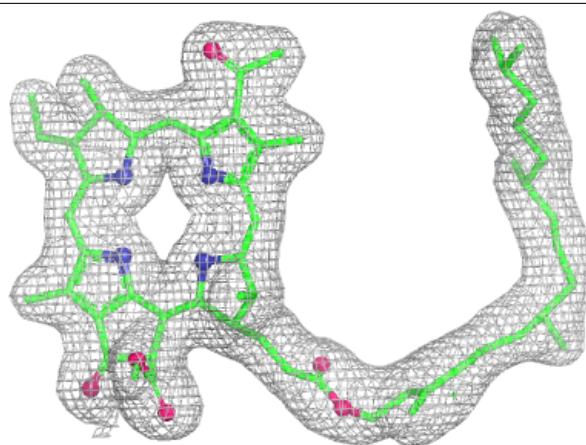
**Electron density around BCB L 401:**

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



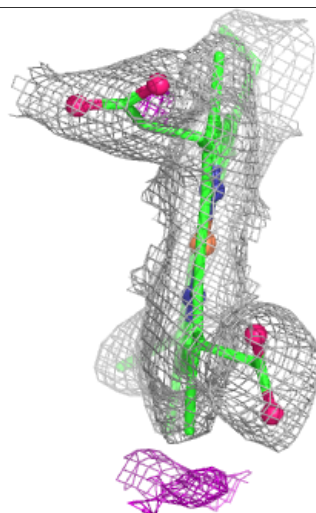
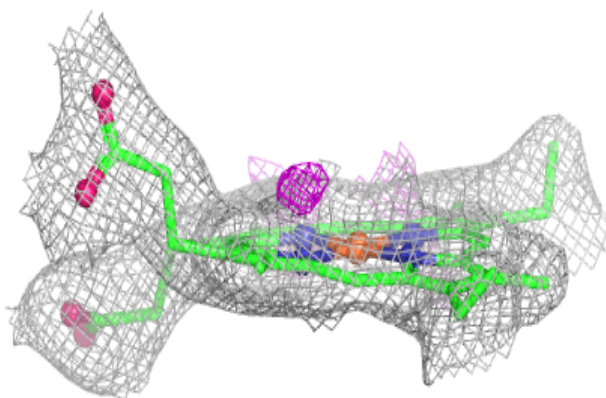
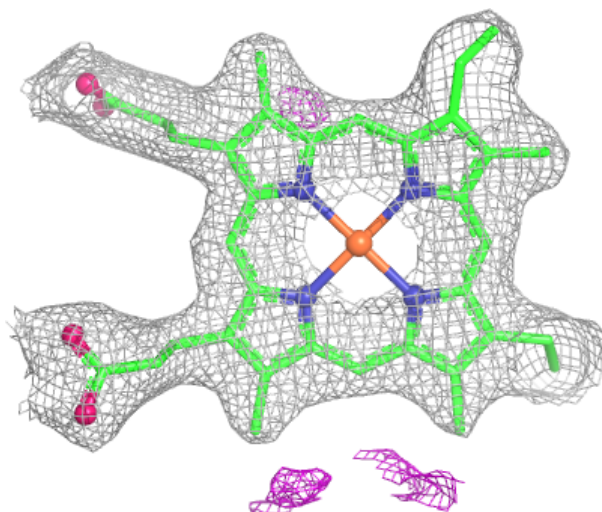
**Electron density around BPB L 402:**

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



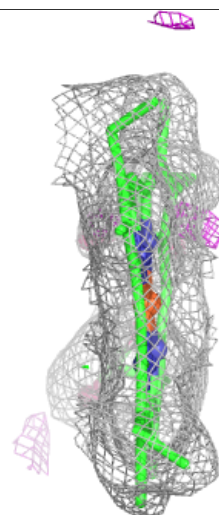
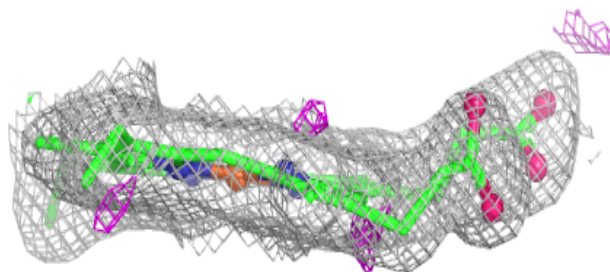
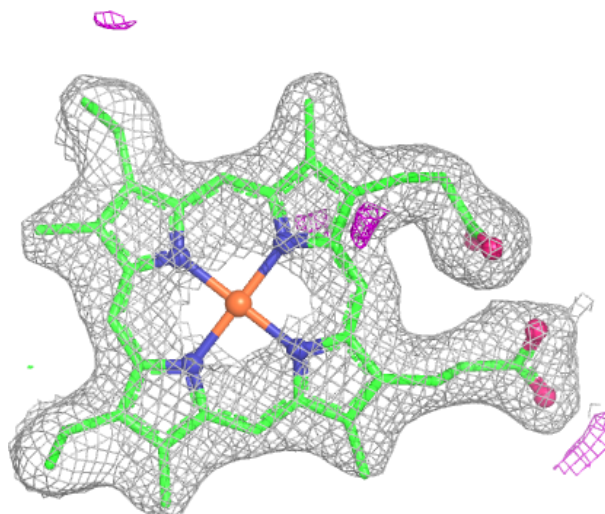
**Electron density around HEC C 401:**

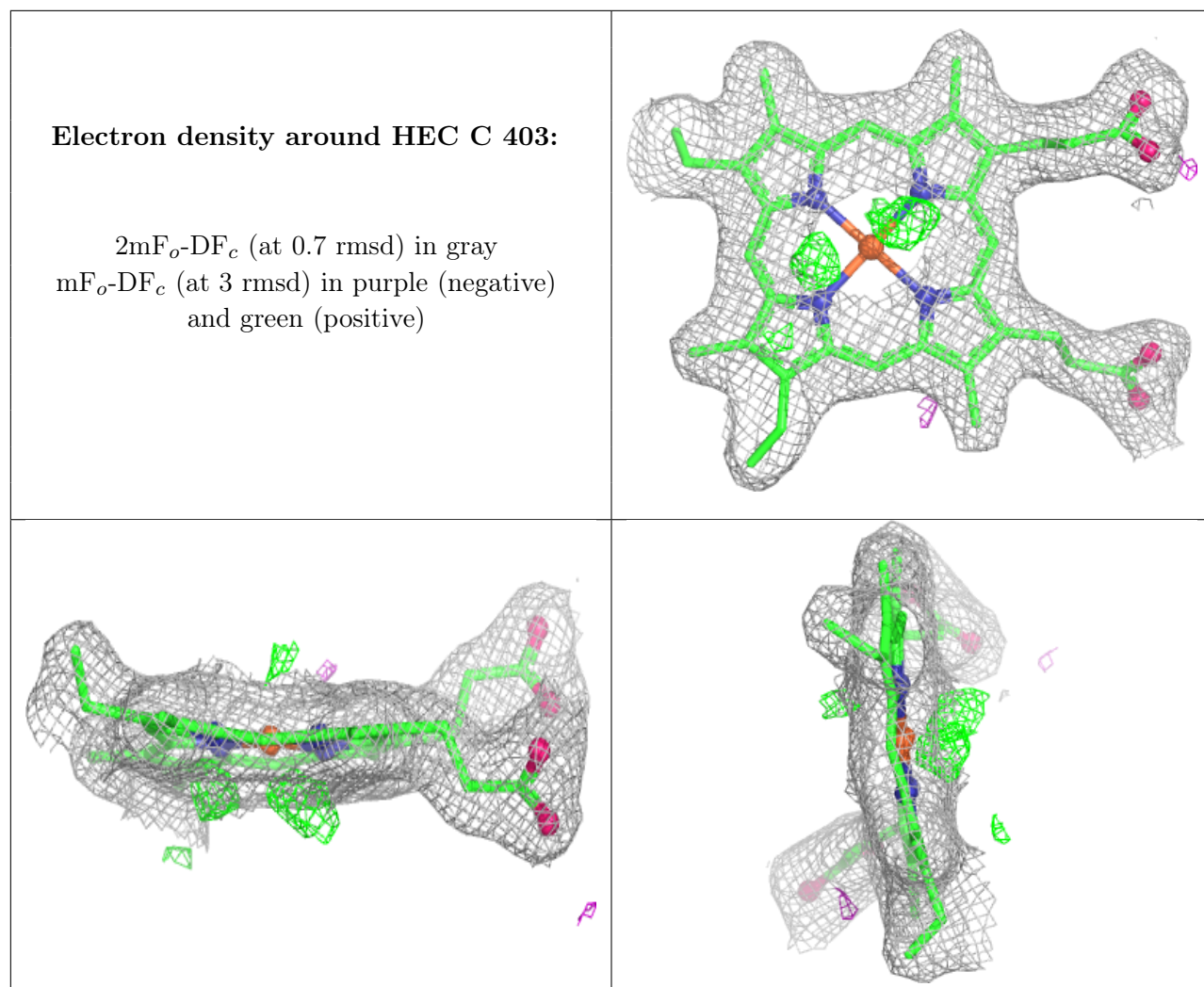
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC C 402:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.